Generative design by using exploration approaches of reinforcement learning in density-based structural topology optimization

2022. 03. 21

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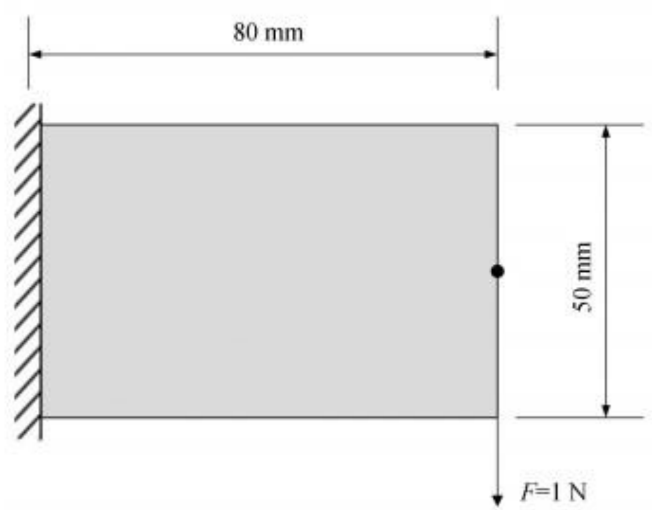
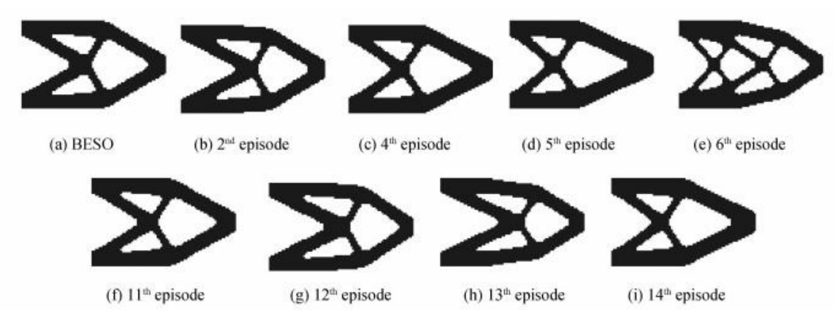
Topology Optimization(TO)

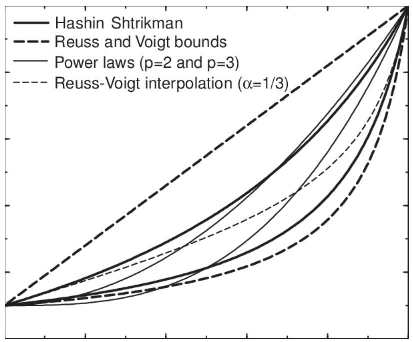
- **About Topology Optimization(TO)**
  - determining the optimal layout of material inside the given design domain
  - Some objective functions :
    I. Structural : Compliance, Weight, Frequency, etc
    II. Thermal : Compliance, Maximum temperature, Temperature variance
  - Constraints : Volume, stress, displacement, etc
  - Considering the difficulty of solving the problem in continuous domain, the design domain is typically discretized into finite elements→ Usually use finite element method

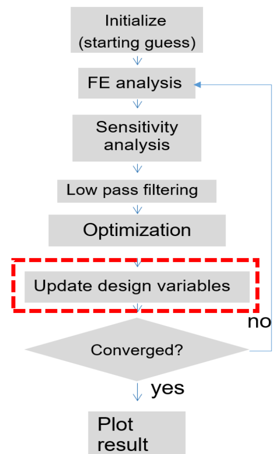




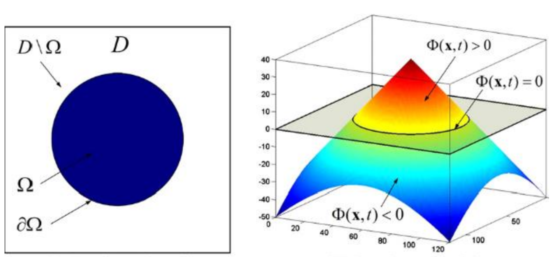
Topology Optimization(TO)

- **Type:**
  - Density based method
    1. SIMP(Solid Isotropic Material Interpolation)
    2. BESO(Bi-Evolutionary Structural Optimization)

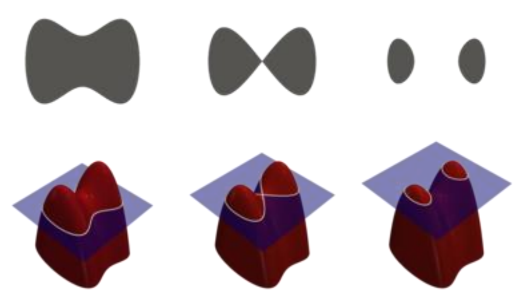




  - Level-set method



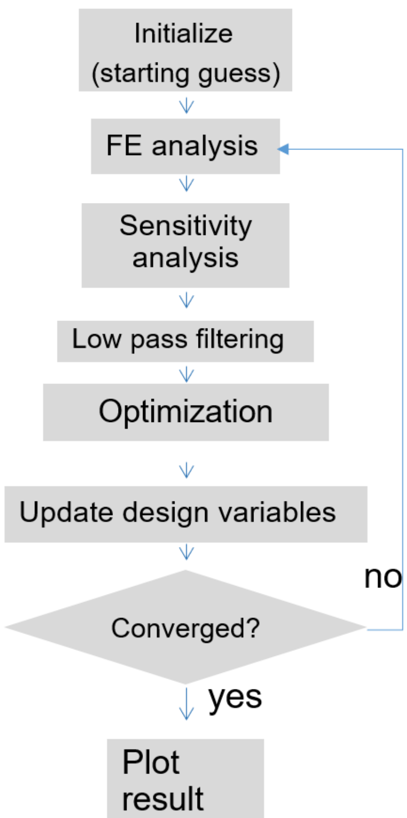
(a) Design domain (b) level set model



Topology Optimization(TO)

- **Topology Optimization(TO)**

Flow chart



Mathematical modeling

Objective : compliance
Constraint : volume

$$\text{Min : } C = \frac{1}{2} f^{\mathrm{T}} u,$$
$$\text{Subject to : } V^* = \sum_{e=1}^{N} V_e x_e,$$
$$x_e = x_{\min} \text{ or } 1 \text{ (BESO)},$$
$$x_e \in [x_{\min}, 1] \text{ (SIMP)}.$$

Topology Optimization(TO)

- **Topology Optimization(TO)**
  - **Updating scheme(Optimality Criteria, OC)**
    - **I. Using duality and Adjoint variable method**

$$x_e^{t+1} = \begin{cases} \max\left(x_{\min},\ x_e^t - m\right) & \text{if } x_e^t B_e^\eta \le \max\left(x_{\min},\ x_e^t - m\right) \\ \min\left(1,\ x_e^t + m\right) & \text{if } \min\left(1,\ x_e^t + m\right) \le x_e^t B_e^\eta \\ x_e^t B_e^\eta & \text{otherwise} \end{cases}$$

$$B_e = \lambda^{-1} p x_e^{p-1} u_e^{\mathrm{T}} K_e u_e,$$

    - **II. For BESO**

$$V_{t+1} = \max\left(V^*,\ V_t\left(1 - ER\right)\right)$$

ER : the evolutionary volume ratio

Using Exploration approaches of Reinforcement Learning in STO

- Naïve Exploration(ε-greedy)
- Optimistic Exploration(Upper Confidence Bound, UCB)
- Probability Matching(Thompson Sampling, TS)
- Information State Search(Information-Directed Search,IDS)

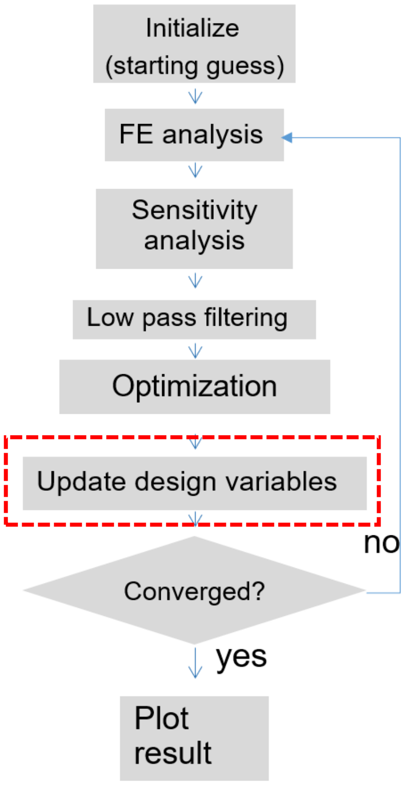
Using Exploration approaches of Reinforcement Learning in STO

- **Naïve Exploration(ε-greedy)**

ε-greedy : $\pi(a|s) \leftarrow \begin{cases} 1-\varepsilon+\frac{\varepsilon}{|A(s)|} & \text{if } a=a^* \\ \frac{\varepsilon}{|A(s)|} & \text{if } a \neq a^* \end{cases}$

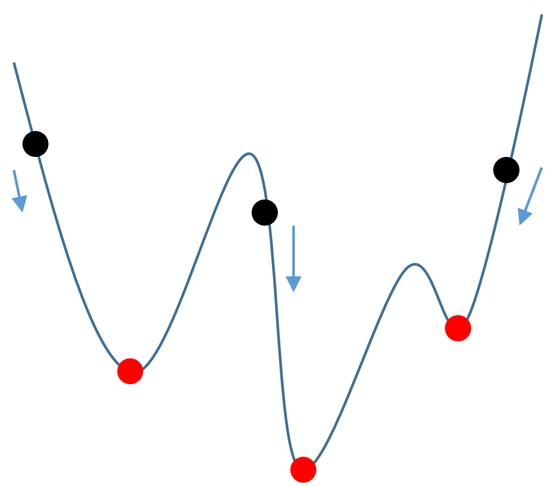
- Used only for BESO method
- Initializes the Q function(action-value) to high value
- Actions : Add or Remove the element density

1. Ranking element sensitivities
2. Dividing into higher and lower class
3. the bottom (1-ε)of the total elements firstly removed
4. ε are removed randomly from the lower class

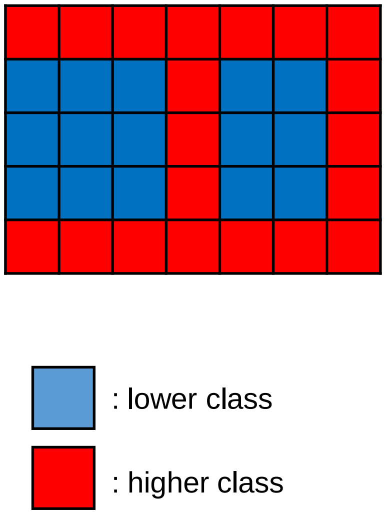


Using Exploration approaches of Reinforcement Learning in STO

- **Naïve Exploration(ε-greedy)**
  - A random perturbation during the process of adding and removing elements is needed
  - Need to prevent the whole structure from collapsing suddenly
    1. Sorting the elements by their sensitivity values
    2. Elements are divided into lower and higher class
    3. The bottom (1-ε) of the total elements which need deleting in this iteration are firstly removed
  - For the convergence, decaying ε-greedy($\varepsilon \leftarrow \varepsilon_0 - \varepsilon_0 (t/t_0)^3$) is used

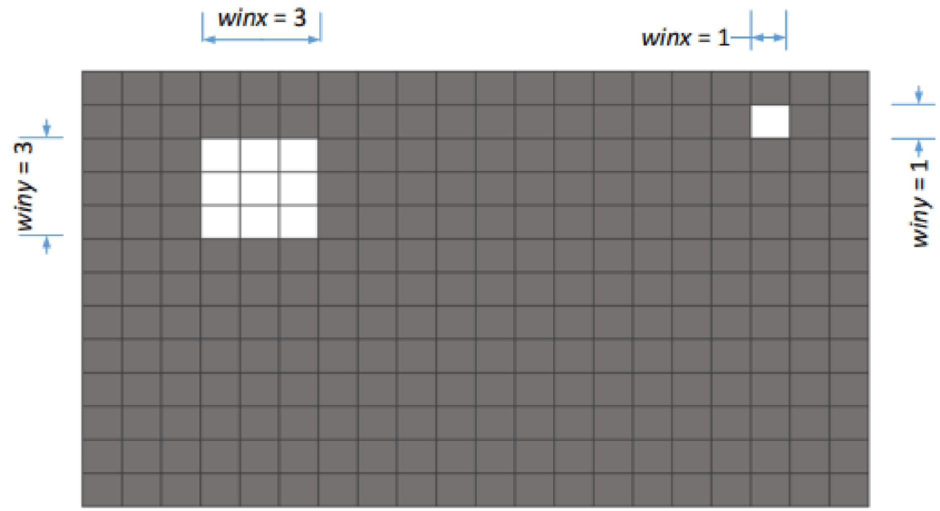


<local minima for each starting point>



Using Exploration approaches of Reinforcement Learning in STO

- **Naïve Exploration(ε-greedy)**
  - Search window
    I. The effect of removing just one element is not obvious
    II. Using search window, the neighbor elements are also deleted at the same time

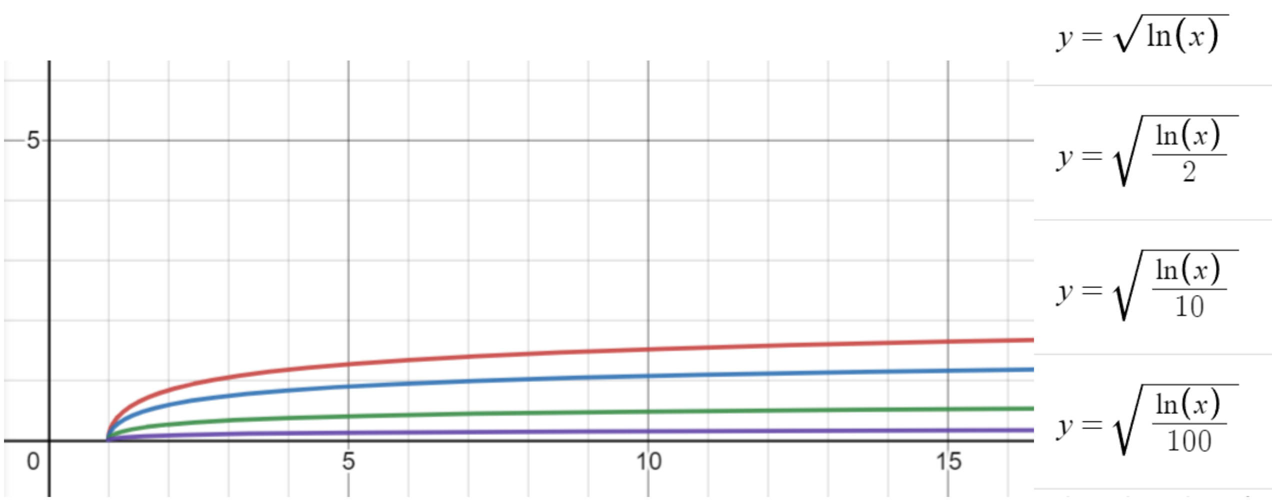


Using Exploration approaches of Reinforcement Learning in STO

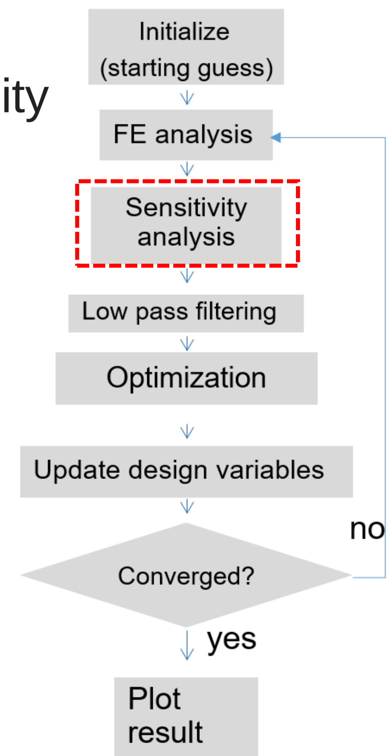
- **Optimistic exploration(upper confidence bound)**

$$A_t = \underset{a}{\operatorname{argmax}} \left[Q_t(a) + cB(a) \right], \qquad B(a) = \sqrt{\frac{2 \ln t}{N(a)}},$$

  - Keeping the balance between the uncertainty and optimality
  - Adopting UCB to calculating the sensitivities



<y=sqrt(ln(x))>



Using Exploration approaches of Reinforcement Learning in STO

- Optimistic exploration(upper confidence bound)
  - **Adopting UCB for TO**

$$A_t = \underset{a}{\operatorname{argmax}} \left[Q_t(a) + cB(a) \right], \qquad B(a) = \sqrt{\frac{2 \ln t}{N(a)}},$$

$$\alpha_t^e = \alpha_t^e - c\sqrt{\frac{ln(t)}{2N\left(a_t^e\right)}}, \qquad \alpha_e = -0.5 p x_e^{p-1} u_e^{\mathrm{T}} K_e u_e,$$

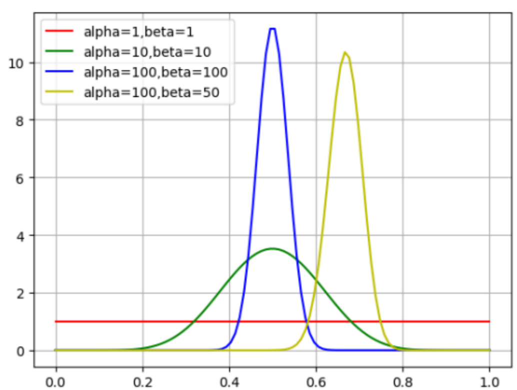
For SIMP : $N\left(a_{t+1}^e\right) = N\left(a_t^e\right) + \max\left(0,\ x_{t+1}^e - x_t^e\right),$

For BESO : $N\left(a_{t+1}^e\right) = N\left(a_t^e\right) + 1\ \ if\ x_{t+1}^e = 1$

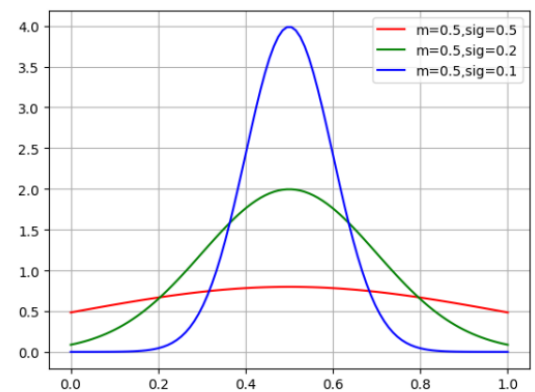
Using Exploration approaches of Reinforcement Learning in STO

- **Probability Matching(Thompson Sampling)**
  - Uses posterior probability to achieve exploration based on Bayesian theory
  - Encourage the exploration of uncertain actions

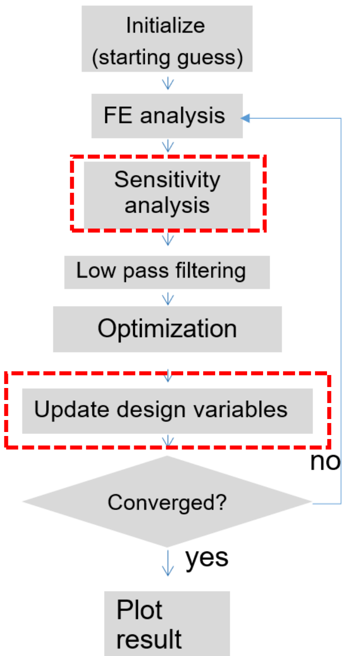
$$\pi(a|h_t) = P[Q(a) > Q(a'),\ \forall a' \neq a \,\big|\, h_t] = E_{R|h_t}[1(a = \underset{a\in A}{\mathrm{argmax}}\, Q(a))]$$



(a) Beta distribution



(b) Gaussian distribution



Using Exploration approaches of Reinforcement Learning in STO

- Probability Matching(Thompson Sampling)

Interactive Real Time Resolution of a Multi Armed Bandit Problem Using Thompson Sampling

Using Exploration approaches of Reinforcement Learning in STO

- **Probability Matching(Thompson Sampling)**
  - Sequence of TS
    I. Sample the reward R from the posterior reward distribution P
    II. Computes the action-value function
    III. Take the optimal action by the policy
    IV. Execute the chosen action in actual environment and get the reward
    V. Update the posterior distribution P

[If selecting Beta distribution] $$(\alpha, \beta) = (\alpha, \beta) + (r_t, 1 - r_t)$$

[If selecting Gaussian distribution]
$$\mu_{t+1,\,a} = \left(\frac{\mu_{t,\,a}}{\sigma_{t,a}^2} + \frac{Y_{t,\,a}}{\sigma_0^2}\right) / \left(\frac{1}{\sigma_{t,a}^2} + \frac{1}{\sigma_0^2}\right)$$
$$\sigma_{t+1,\,a} = \left(\frac{1}{\sigma_{t,a}^2} + \frac{1}{\sigma_0^2}\right)^{-1}$$

  - Define reward function
    I. Defined as the rank of the sensitivity numbers of elements
    II. 0 to 1 from higher sensitivity to lower sensitivity

Using Exploration approaches of Reinforcement Learning in STO

- **Information State search(Information-directed search)**
  - Information state search views information as a part of state

$$a = \underset{a}{\operatorname{argmin}} \frac{\Delta(a)^2}{g(a)} \tag{1}$$

$$\Delta(a) = E[r(a^*) - r(a))]$$

$$g_t(a) = E[H(\gamma_t) - H(\gamma_{t+1}) \big| h_t,\ A_t = a]$$
$$\gamma_t(a) = P(A^* = a \big| h_t)$$

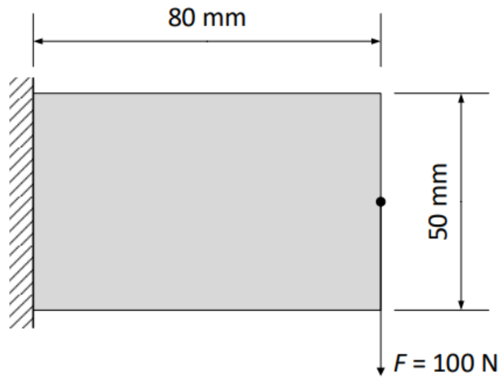
  - Sequence
    I. Get the samples for estimation by interacting with the actual environment in the first iteration, and by the updated posterior reward distribution P in the following steps
    II. Compute Δ, g and the information gain ratio
    III. Take the optimal action by Equation (1)
    IV. Execute the chosen action in actual environment and get the reward
    V. Update the posterior reward distribution by Equation of Beta and Gaussian distribution

Using Exploration approaches of Reinforcement Learning in STO

- **Information State search(Information-directed search)**
  - High-dimensional problem
    - I. reward is the same as Thompson sampling
    - II. proceed the STO by BESO in the first episode
    - III. divide the elements by the rank of sensitivity numbers into 10 to 20 groups
    - IV. each group is corresponding to one action which can be chosen for a certain times equal to the number of solid element it contains
    - V. In the following episodes, the number of elements that need deleting in each group will be allocated by IDS first
    - VI. the elements in each group are chosen by sampling according to the actual reward function of each element.

Cases and Discussion

- Cantilever Beam



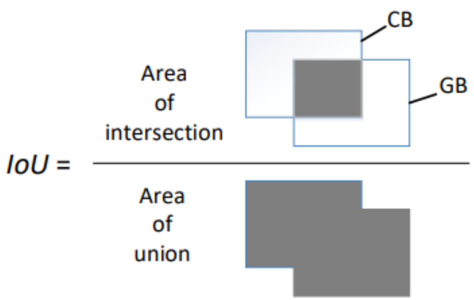
E = 1MPa
nu = 0.3(Poisson's ratio)
Volume fraction = 50%
ER(BESO) = 0.04
Move limit(SIMP) = 0.2
Filter radius = 4mm
Convergence criteria =

$$\frac{\left|\sum_{i=1}^{M}(C_{t-i+1} - C_{t-M-i+1})\right|}{\sum_{i=1}^{M} C_{t-i+1}} \leq$$

0.1%(BESO)
1%(SIMP)

M = 5

$$IoU = \frac{area(CB) \cap \ area(GB)}{area(CB) \cup \ area(GB)}.$$



Cases and Discussion

- Cantilever Beam

ε-greedy

UCB-BESO

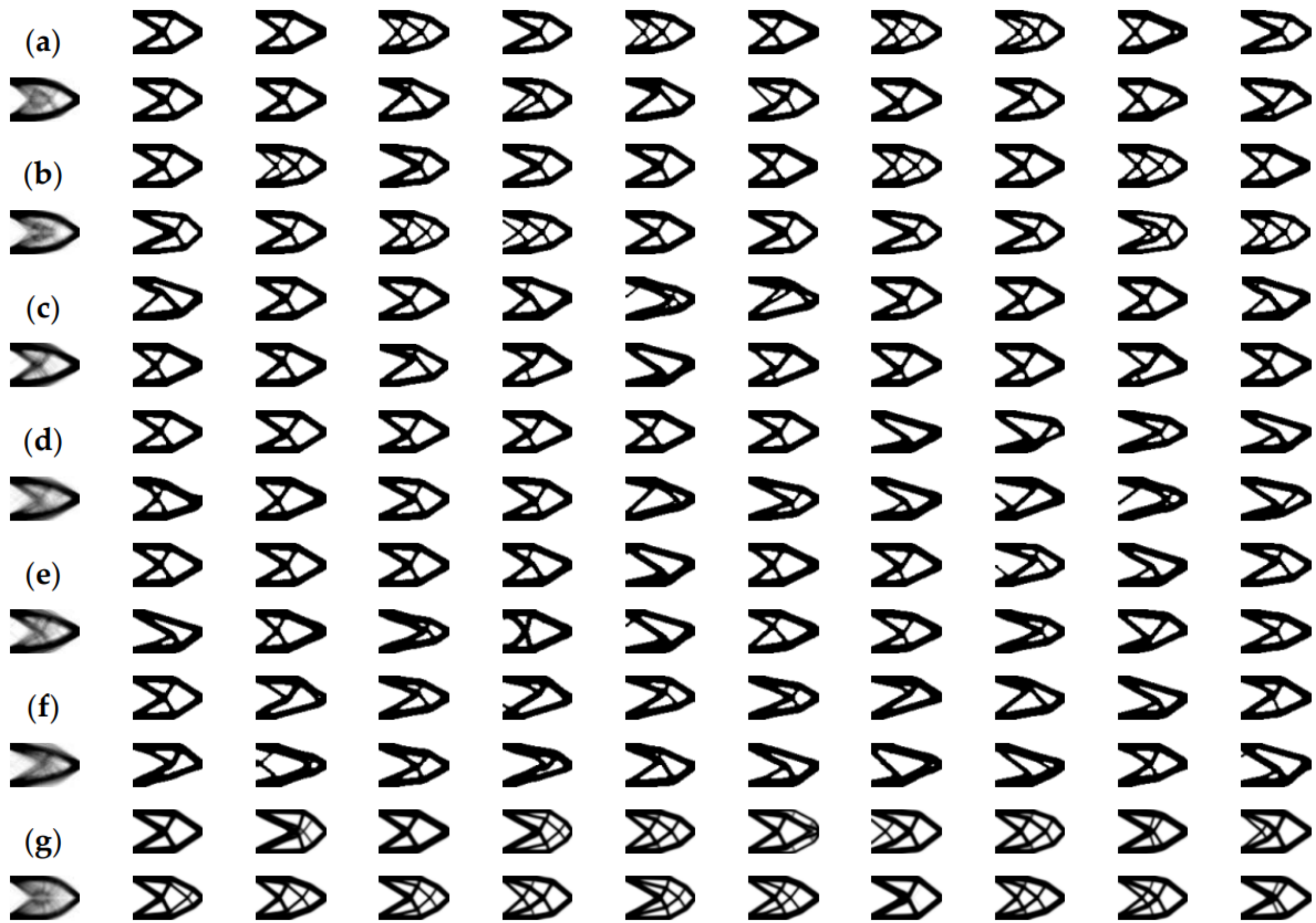
TS(beta)-BESO

TS(Gaussian)-BESO

VIDS(beta)-BESO

IDS(Gaussian)-BESO

UCB-SIMP



Cases and Discussion

- Cantilever Beam

Table 1. Calculation results of the cantilever beam by UCB with BESO.

Nth Episode	*C* (10^5 N·mm)	*IOU*	*ITER*	*Nth* Episode	*C* (10^5 N·mm)	*IOU*	*ITER*
BESO	1.873		26	11	1.923	0.736	43
2	1.891	0.600	28	12	1.878	0.851	34
3	1.918	0.779	24	13	1.873	0.740	46
4	1.885	0.794	55	14	1.912	0.801	34
5	1.883	0.856	24	15	1.876	0.896	29
6	1.883	0.695	37	16	1.881	0.858	26
7	1.877	0.746	31	17	1.913	0.866	75
8	1.867	0.859	41	18	1.900	0.894	42
9	1.878	0.870	28	19	1.963	0.719	100
10	1.891	0.868	30	20	1.886	0.893	40

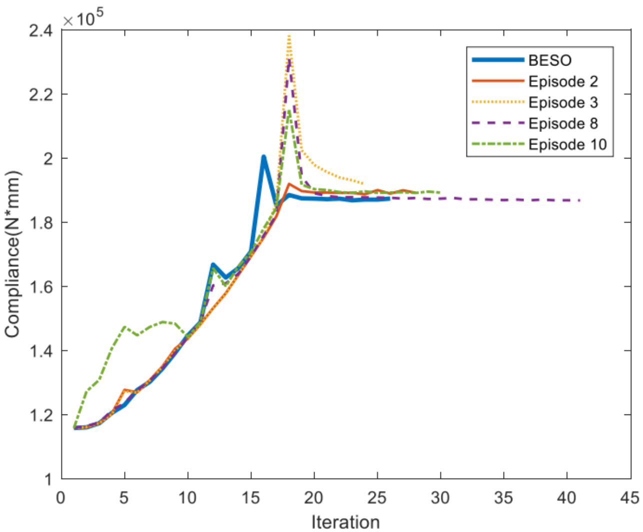
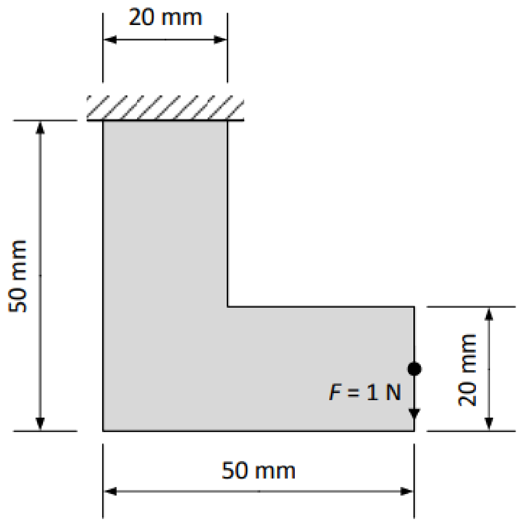


Figure 7. Evolutionary histories of the compliance for the cantilever beam by UCB with BESO.

Cases and Discussion

- L-shaped Beam



E = 1MPa
nu = 0.3(Poisson's ratio)
Volume fraction = 50%
ER(BESO) = 0.03
Move limit(SIMP) = 0.2
Filter radius = 1.5mm
Convergence criteria =

$$\frac{\left|\sum_{i=1}^{M}(C_{t-i+1} - C_{t-M-i+1})\right|}{\sum_{i=1}^{M} C_{t-i+1}} \leq \begin{matrix} 1\%(\text{BESO}) \\ 0.01\%(\text{SIMP}) \end{matrix}$$

M = 5

Cases and Discussion

- Cantilever Beam

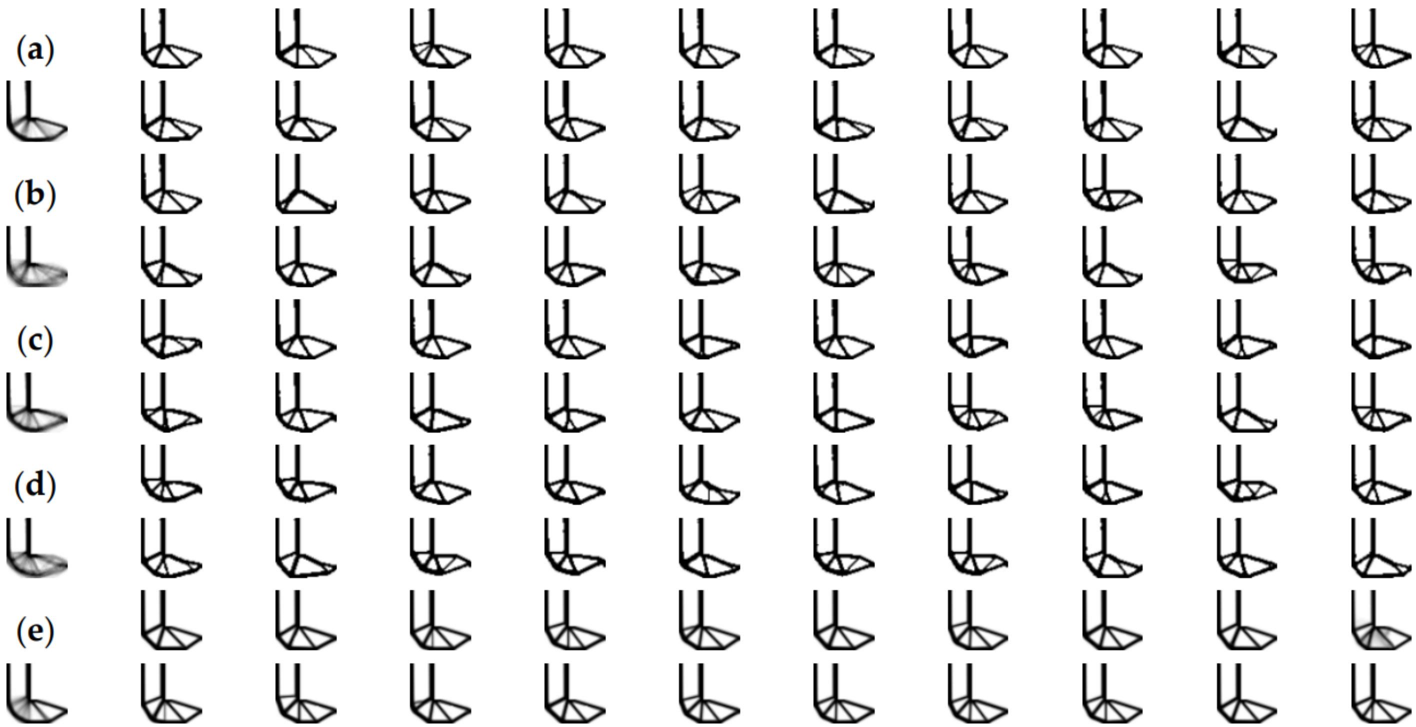
ε-greedy

UCB-BESO

TS(beta)-BESO

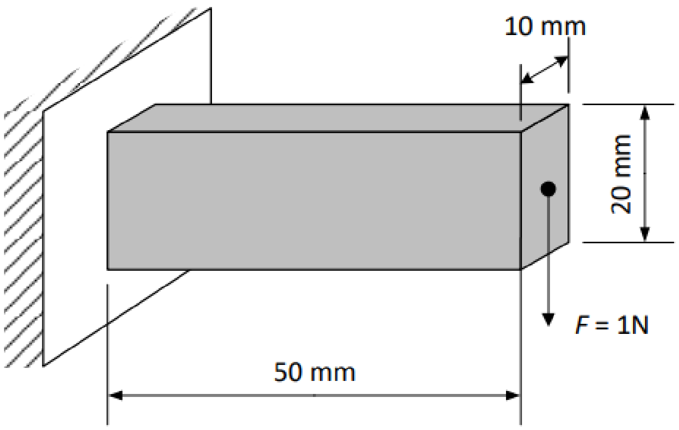
TS(Gaussian)-BESO

UCB-SIMP



Cases and Discussion

- **3D Cantilever Beam**



E = 1MPa
nu = 0.3(Poisson's ratio)
Volume fraction = 50%
ER(BESO) = 0.03
Move limit(SIMP) = 0.2
Filter radius = 1.5mm
Convergence criteria =

$$\frac{\left|\sum_{i=1}^{M}(C_{t-i+1} - C_{t-M-i+1})\right|}{\sum_{i=1}^{M} C_{t-i+1}} \leq \begin{array}{l} 1\%(\text{BESO}) \\ 0.01\%(\text{SIMP}) \end{array}$$

M = 5

Cases and Discussion

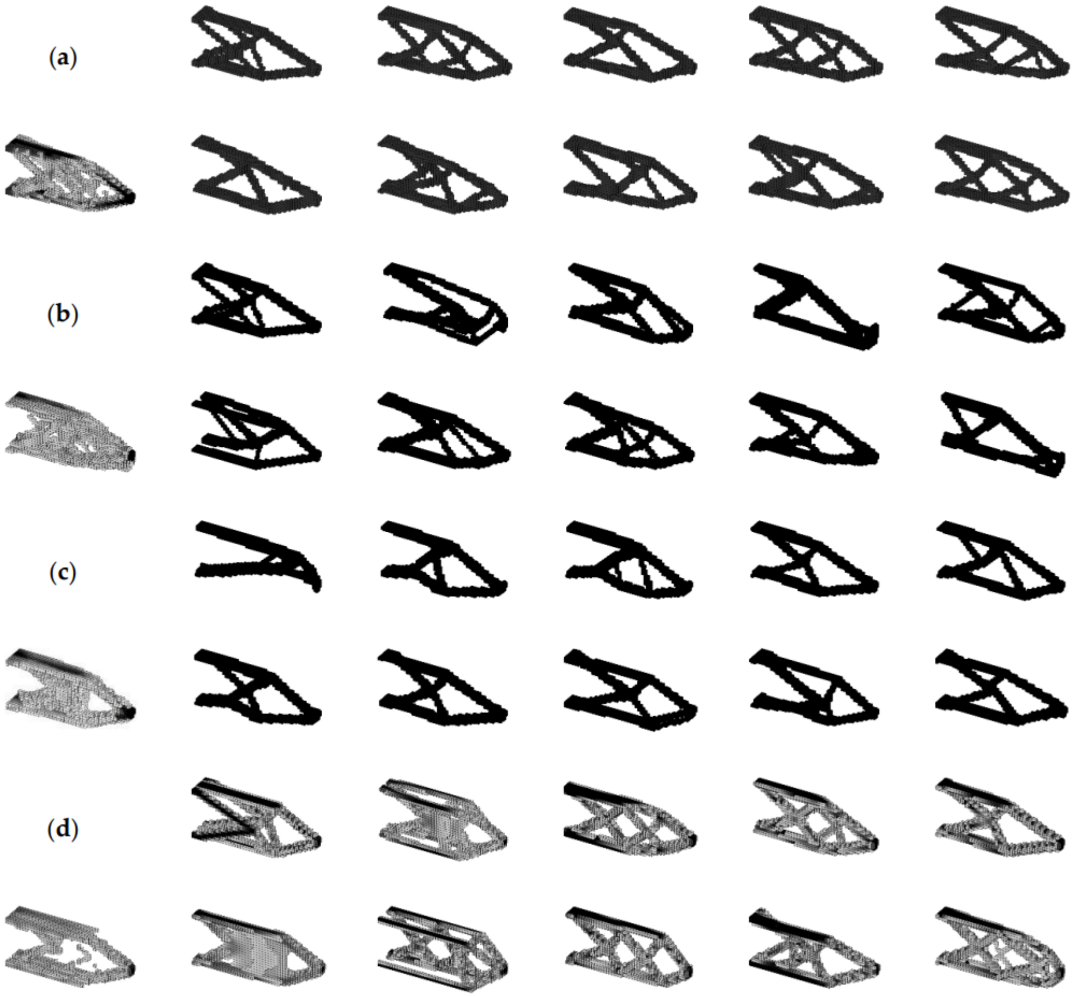
- **3D Cantilever Beam**

ε-greedy

UCB-BESO

TS(beta)-BESO

UCB-SIMP



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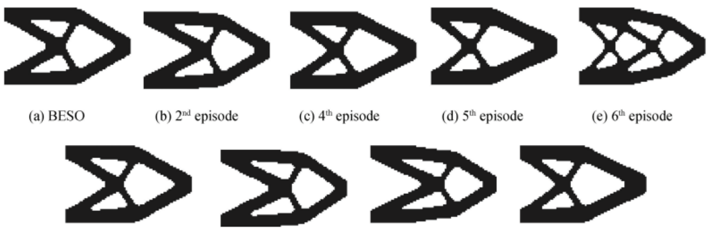
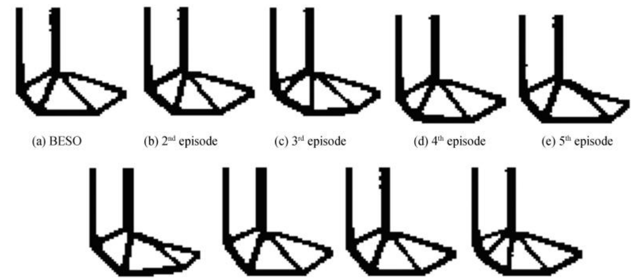


(a) BESO (b) 2nd episode (c) 4th episode (d) 5th episode (e) 6th episode

(f) 11th episode (g) 12th episode (h) 13th episode (i) 14th episode

strikethrough)

*N*th episode	C(N · mm)	ΔC(%)	IoU	ITER	Acceptability (Yes or No)
BESO	18.73			26	
2	18.77	0.20	0.832	23	Yes
3	18.75	0.09	~~0.938~~	30	No
4	18.79	0.33	0.741	35	Yes
5	18.99	1.40	0.773	42	Yes
6	18.88	0.82	0.621	27	Yes
7	18.76	0.16	~~0.929~~	28	No
8	18.72	−0.05	~~0.979~~	34	No
9	18.70	−0.17	~~0.931~~	28	No
10	18.97	1.31	~~0.978~~	39	No
11	18.68	−0.26	0.881	28	Yes
12	18.82	0.48	0.863	37	Yes
13	18.96	1.25	0.838	32	Yes
14	18.83	0.54	0.895	34	Yes



(a) BESO (b) 2nd episode (c) 3rd episode (d) 4th episode (e) 5th episode

(f) 6th episode (g) 7th episode (h) 8th episode (i) 9th episode

*N*th episode	C (N · mm)	ΔC(%)	IoU	ITER	Accept-ability
BESO	102.26			52	
2	101.77	−0.48	0.776	63	Yes
3	102.29	0.03	0.712	64	Yes
4	102.86	0.58	0.835	53	Yes
5	103.86	1.57	0.641	97	Yes
6	104.81	2.50	0.645	71	Yes
7	102.25	−0.01	0.766	38	Yes
8	101.77	−0.48	0.830	85	Yes
9	100.78	−1.45	0.795	64	Yes

Thank you for your attention

99line topology optimization(FE analysis)

Stiffness matrix

```
k=[ 1/2-nu/6 1/8+nu/8 -1/4-nu/12 -1/8+3*nu/8 ...
      -1/4+nu/12 -1/8-nu/8 nu/6 1/8-3*nu/8];
   KE = E/(1-nu^2)*[ k(1) k(2) k(3) k(4) k(5) k(6) k(7) k(8)
      k(2) k(1) k(8) k(7) k(6) k(5) k(4) k(3)
      k(3) k(8) k(1) k(6) k(7) k(4) k(5) k(2)
      k(4) k(7) k(6) k(1) k(8) k(3) k(2) k(5)
      k(5) k(6) k(7) k(8) k(1) k(2) k(3) k(4)
      k(6) k(5) k(4) k(3) k(2) k(1) k(8) k(7)
      k(7) k(4) k(5) k(2) k(3) k(8) k(1) k(6)
      k(8) k(3) k(2) k(5) k(4) k(7) k(6) k(1)];
```

Stiffness matrix derived by Appendix code

```
K =

[     (E*(v - 3))/(6*(v^2 - 1)),              -E/(8*(v - 1)),   (E*(v + 3))/(12*(v^2 - 1)), -(E*(3*v - 1))/(8*(v^2 - 1)),  -(E*(v - 3))/(12*(v^2 - 1)),               E/(8*(v - 1)),         -(E*v)/(6*(v^2 - 1)),  (E*(3*v - 1))/(8*(v^2 - 1))]
[              -E/(8*(v - 1)),    (E*(v - 3))/(6*(v^2 - 1)),  (E*(3*v - 1))/(8*(v^2 - 1)),         -(E*v)/(6*(v^2 - 1)),               E/(8*(v - 1)),  -(E*(v - 3))/(12*(v^2 - 1)), -(E*(3*v - 1))/(8*(v^2 - 1)),   (E*(v + 3))/(12*(v^2 - 1))]
[   (E*(v + 3))/(12*(v^2 - 1)),  (E*(3*v - 1))/(8*(v^2 - 1)),    (E*(v - 3))/(6*(v^2 - 1)),               E/(8*(v - 1)),         -(E*v)/(6*(v^2 - 1)), -(E*(3*v - 1))/(8*(v^2 - 1)),  -(E*(v - 3))/(12*(v^2 - 1)),              -E/(8*(v - 1))]
[ -(E*(3*v - 1))/(8*(v^2 - 1)),         -(E*v)/(6*(v^2 - 1)),               E/(8*(v - 1)),    (E*(v - 3))/(6*(v^2 - 1)),  (E*(3*v - 1))/(8*(v^2 - 1)),   (E*(v + 3))/(12*(v^2 - 1)),              -E/(8*(v - 1)),  -(E*(v - 3))/(12*(v^2 - 1))]
[  -(E*(v - 3))/(12*(v^2 - 1)),               E/(8*(v - 1)),         -(E*v)/(6*(v^2 - 1)),  (E*(3*v - 1))/(8*(v^2 - 1)),    (E*(v - 3))/(6*(v^2 - 1)),              -E/(8*(v - 1)),   (E*(v + 3))/(12*(v^2 - 1)), -(E*(3*v - 1))/(8*(v^2 - 1))]
[               E/(8*(v - 1)),  -(E*(v - 3))/(12*(v^2 - 1)), -(E*(3*v - 1))/(8*(v^2 - 1)),   (E*(v + 3))/(12*(v^2 - 1)),              -E/(8*(v - 1)),    (E*(v - 3))/(6*(v^2 - 1)),  (E*(3*v - 1))/(8*(v^2 - 1)),         -(E*v)/(6*(v^2 - 1))]
[         -(E*v)/(6*(v^2 - 1)), -(E*(3*v - 1))/(8*(v^2 - 1)),  -(E*(v - 3))/(12*(v^2 - 1)),              -E/(8*(v - 1)),   (E*(v + 3))/(12*(v^2 - 1)),  (E*(3*v - 1))/(8*(v^2 - 1)),    (E*(v - 3))/(6*(v^2 - 1)),               E/(8*(v - 1))]
[  (E*(3*v - 1))/(8*(v^2 - 1)),   (E*(v + 3))/(12*(v^2 - 1)),              -E/(8*(v - 1)),  -(E*(v - 3))/(12*(v^2 - 1)), -(E*(3*v - 1))/(8*(v^2 - 1)),         -(E*v)/(6*(v^2 - 1)),               E/(8*(v - 1)),    (E*(v - 3))/(6*(v^2 - 1))]
```

Appendix

Objective

$$\min_{x} c(x) = U^T K U = \sum_{e=1}^{N} (x_e)^p {u_e}^T k_0 u_e$$

Subject to

$V(x) = fV_0$

$KU = F$

$0 < x_{min} \leq x \leq 1$

Lagrangian function - KKT condition.

$$L = c(x) + \lambda(V(x) - fV_0) + {\lambda_1}^T(KU - F) + \sum_{e=1}^{N} \lambda_{2e}(x_{min} - x_e) + \sum_{e=1}^{N} \lambda_{3e}(x_e - x_{max})$$

Appendix

- $L = c(x) + \lambda(V(x) - fV_0) + {\lambda_1}^T(KU - F) + \sum_{e=1}^{N} \lambda_{2e}(x_{min} - x_e) + \sum_{e=1}^{N} \lambda_{3e}(x_e - x_{max})$

$$\frac{\partial L}{\partial x_e} = \frac{\partial U^T}{\partial x_e} KU + U^T \frac{\partial K}{\partial x_e} U + U^T K \frac{\partial U}{\partial x_e} + \lambda \frac{\partial V}{\partial x_e} + {\lambda_1}^T (\frac{\partial K}{\partial x_e} U + K \frac{\partial U}{\partial x_e}) - \lambda_{2e} + \lambda_{3e} = 0$$

- $\frac{\partial F}{\partial x_e} = 0$ (independent with design variable)
- $\lambda_{2e} = \lambda_{3e} = 0$
  (Lagrangian multiplier is zero when the design variable value is in the boundary value .)
- Adjoint method

$$\frac{dL}{dx_e} = \frac{\partial c}{\partial x_e} + \frac{\partial c}{\partial u}\frac{du}{dx_e} + {\lambda_1}^T (\frac{\partial k}{\partial x_e} u + k \frac{du}{dx_e})$$

to erase $\frac{du}{dx_e}$ -> ${\lambda_1}^T = -2u^T$

$k = (x_e)^p k_0$ based on SIMP method(Solid Isotropic Microstructure with penalty).

$$\frac{\partial L}{\partial x_e} = -p(x_e)^{p-1} U^T k_0 U + \lambda \frac{\partial V}{\partial x_e} = 0$$

$$U^T k_0 U > 0 \text{ and } \frac{\partial V}{\partial x_e} = v_e = 1 > 0$$

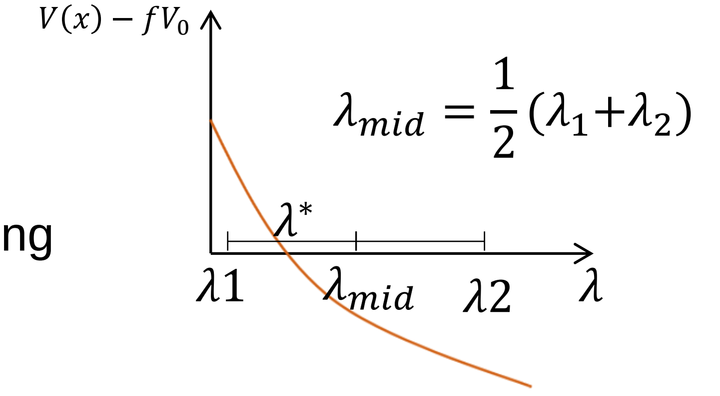
Lagrangian multiplier should have only one value.

Appendix

- $\dfrac{p({x_e}^*)^{p-1}U^T k_0 U}{\lambda\frac{\partial V}{\partial x_e}} = {B_e}^* = 1$

to find out λ. Use bi-sectioning algorithm

${x_e}^{k+1} = {x_e}^k({B_e}^k)^{\eta}$ η=numerical damping



$if\ V(x^{k+1}) - fV_0 < 0, \quad \lambda^* < \lambda_{mid}$

$\lambda_2 = \lambda_{mid}$

$if\ V(x^{k+1}) - fV_0 > 0, \quad \lambda^* > \lambda_{mid}$

$\lambda_1 = \lambda_{mid}$

$$x_e^{\text{new}} = \begin{cases} \max(x_{\min}, x_e - m) \\ \quad \text{if} \quad x_e B_e^\eta \le \max(x_{\min}, x_e - m), \\ x_e B_e^\eta \\ \quad \text{if} \quad \max(x_{\min}, x_e - m) < x_e B_e^\eta < \min(1, x_e + m), \\ \min(1, x_e + m) \\ \quad \text{if} \quad \min(1, x_e + m) \le x_e B_e^\eta, \end{cases}$$