The New Space Mapping Algorithms (since 2000)

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SMSMEO-06

Objectives of Space Mapping

- Optimization of very expensive models
- Construct easy-to-calculate surrogate models

We assume two models of a physical object are available:

- an accurate fine model (expensive)
- a simpler coarse model (cheap)

Type of Problem Considered

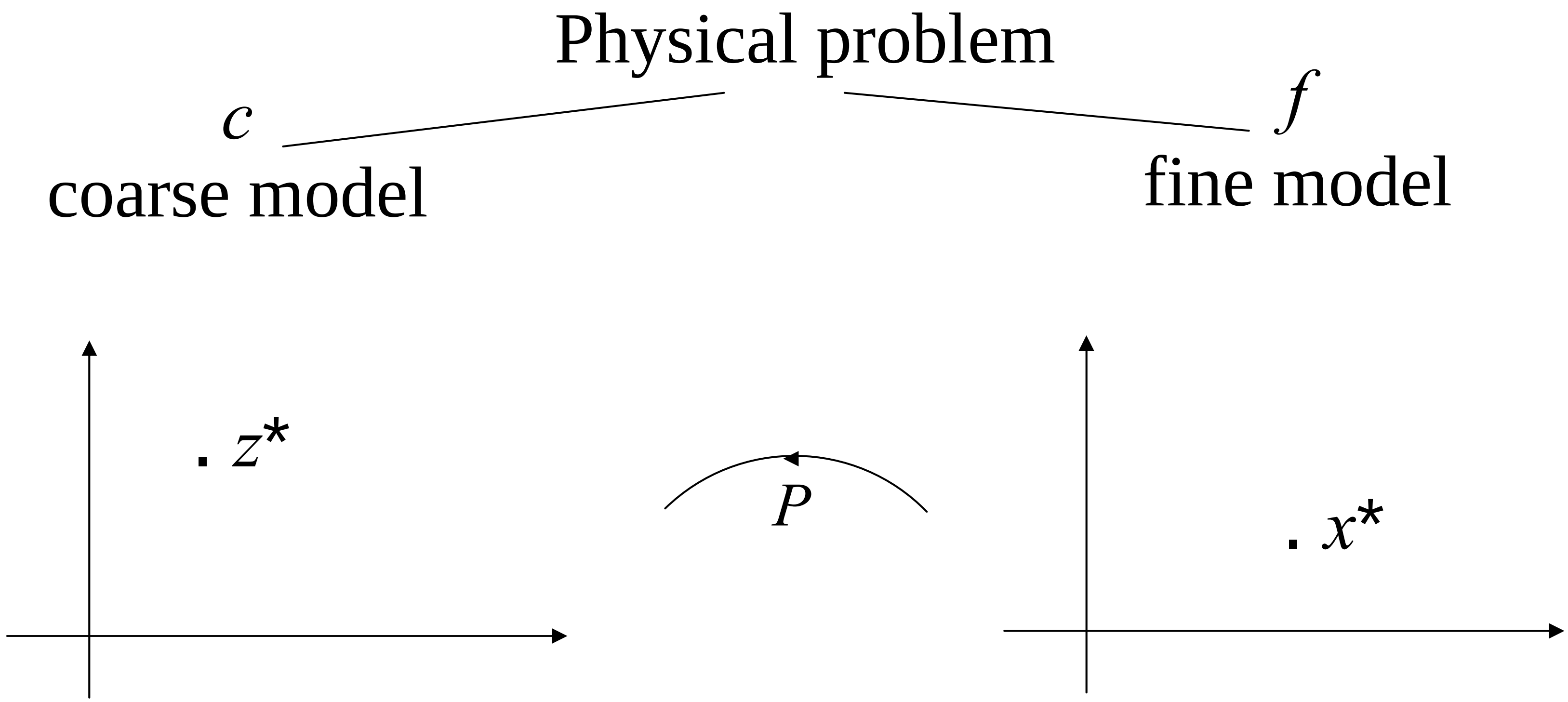
Minimize w.r.t. $x \in \mathrm{R}^n$ the absolute values of the deviations between response $r(x;t_i)$ and specifications y_i

$$f_i(x) = r(x;t_i) - y_i, \quad i = 1, \ldots, m$$

Find $$x^* \in \arg\min_x \{H(f(x))\}$$

Original SM for Optimization

(*Bandler et al., 1995*)



Connect similar responses

$$f(x) \approx c(P(x))$$

Original SM for Optimization

Problem: minimize $H(f(x))$

SM strategy: minimize $H(c(P(x)))$

SM methodology:

For $i = 0,1,2, \ldots$, find estimates $P^{(i)}$ of P and

minimize $H(c(P^{(i)}(x)))$

Original SM: Basic Algorithm

Find initial estimate $x^{(0)}$ to x^{*}

for $i = 0, 1, 2, \ \ldots$ do

calculate $f(x^{(i)})$

find $P(x^{(i)})$

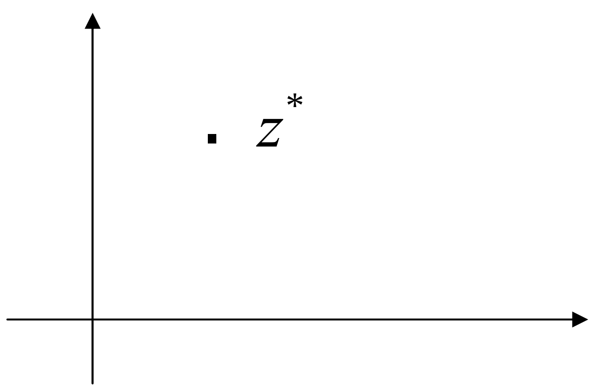
based on previous points find an estimate $P^{(i)}$ of P

minimize $H(c(P^{(i)}(x)))$ to find $x^{(i+1)}$

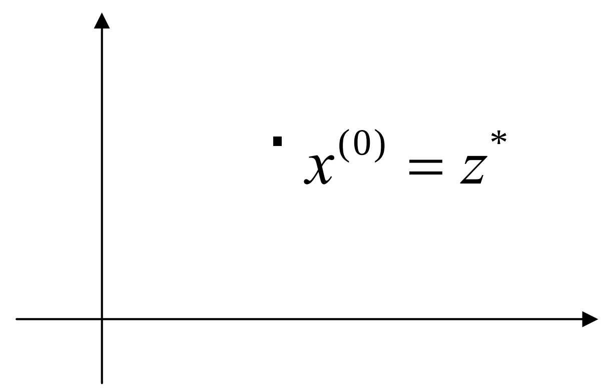
enddo

Initialization

c
coarse model



f
fine model

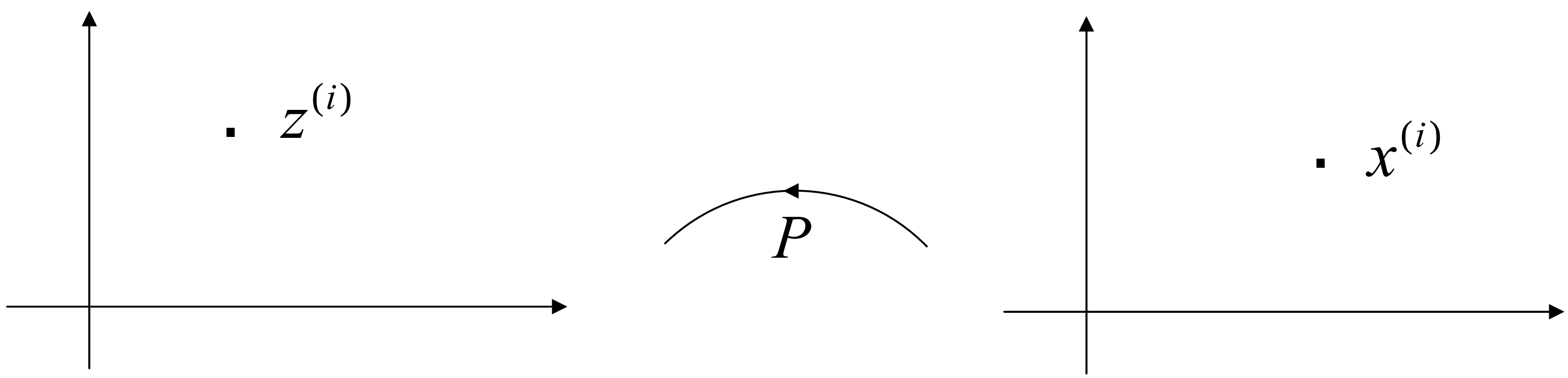


Find the coarse model solution z^*

Find the Space Mapping *P*

c
coarse model

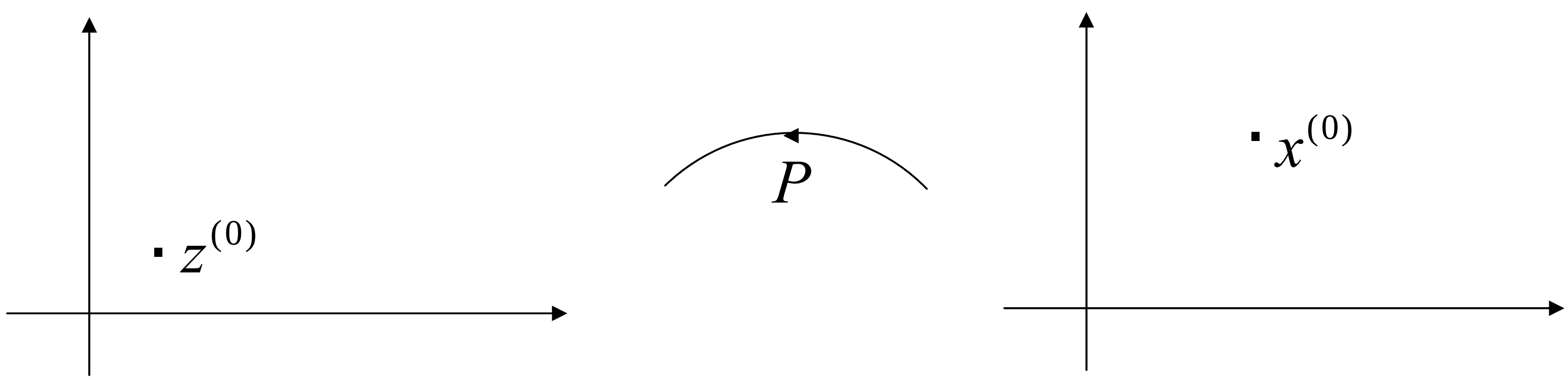
f
fine model



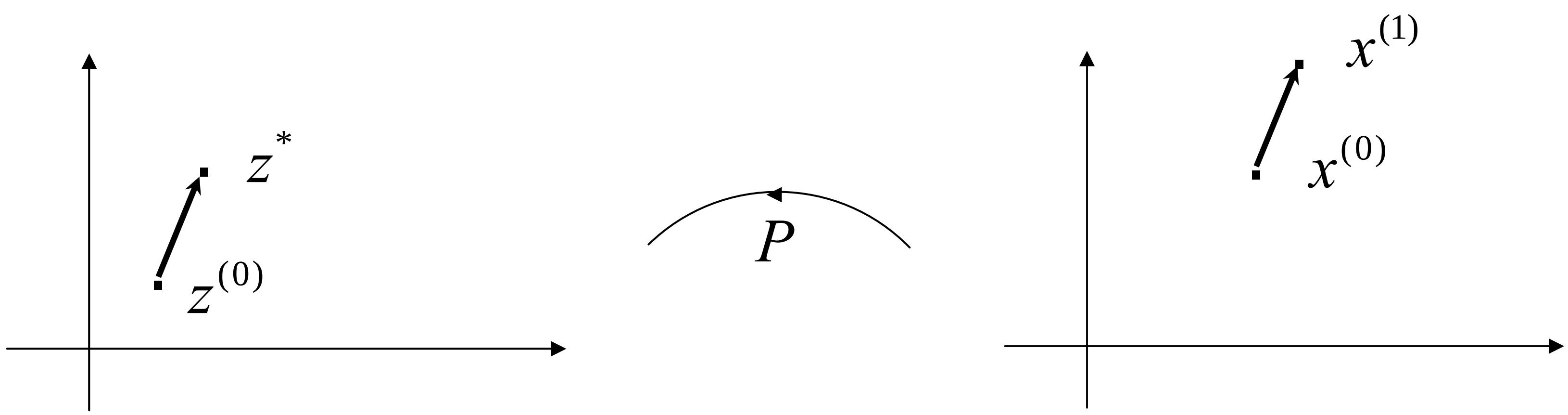
– by connecting similar responses

Parameter Extraction: Find $x^{(0)}$

$$z^{(0)} = P(x^{(0)}) \equiv \arg\min_{z} \left\{ \left\| f(x^{(0)}) - c(z) \right\| \right\}$$



Find $x^{(1)}$



Intuition: $x^{(1)} = x^{(0)} + (z^* - z^{(0)})$

We assume $f(x) \approx c(P(x))$, *i.e.*, $P(x^*) = z^*$

$$P(x) \approx P(x^{(0)}) + J_P(x^{(0)})(x - x^{(0)})$$

$$P^{(0)}(x) \equiv P(x^{(0)}) + B^{(0)}(x - x^{(0)}) \;, \qquad B^{(0)} = I$$

$$x^{(1)} = \arg\min_{x} \left\{ H(c(P^{(0)}(x))) \right\}$$

$$P^{(0)}(x) = z^* \quad \Rightarrow P(x^{(0)}) + (x - x^{(0)}) = z^*$$

$$\Rightarrow \quad z^{(0)} + (x - x^{(0)}) = z^*$$

$$\Rightarrow \quad x^{(1)} = x = x^{(0)} + (z^* - z^{(0)})$$

Original SM Algorithm

$$x^{(0)} = z^*$$

for $i = 0, 1, 2, \ldots$ (while *not* *STOP*) do

calculate $f(x^{(i)})$

$$z^{(i)} = P(x^{(i)}) \equiv \arg\min_{z} \left\{ \left\| f(x^{(i)}) - c(z) \right\| \right\}$$

compute $P^{(i)}$ from $P(x^{(i)})$ and $B^{(i)}$

$$x^{(i+1)} = \arg\min_{x} \left\{ H(c(P^{(i)}(x))) \right\}$$

enddo

Bandler, Biernacki, Chen, Hemmers, Madsen (1995)

i'th Iteration: Estimate *P*

Assume P has been computed at $x^{(0)}, x^{(1)}, \ldots, x^{(i)}$

$$P(x) \approx P(x^{(i)}) + J_P(x^{(i)})(x - x^{(i)})$$

$$P^{(i)}(x) \equiv P(x_f^{(i)}) + B^{(i)}(x - x^{(i)})$$

where $B^{(i)} \approx J_P(x^{(i)})$ is, e.g., a Broyden update

Traditional Taylor-based Optimization

At the iterate $x^{(i)}$ minimize $H(s_T^{(i)}(x))$

where $s_T^{(i)}$ is a first order Taylor estimate of f at $x^{(i)}$

Combined surrogate:

$$s_{comb}^{(i)}(x) = \eta_i s_T^{(i)}(x) + (1-\eta_i) s_{SM}^{(i)}(x), \qquad 0 \le \eta_i \le 1$$

Bandler, Bakr, Madsen, Søndergaard (2001)

Approximation Errors

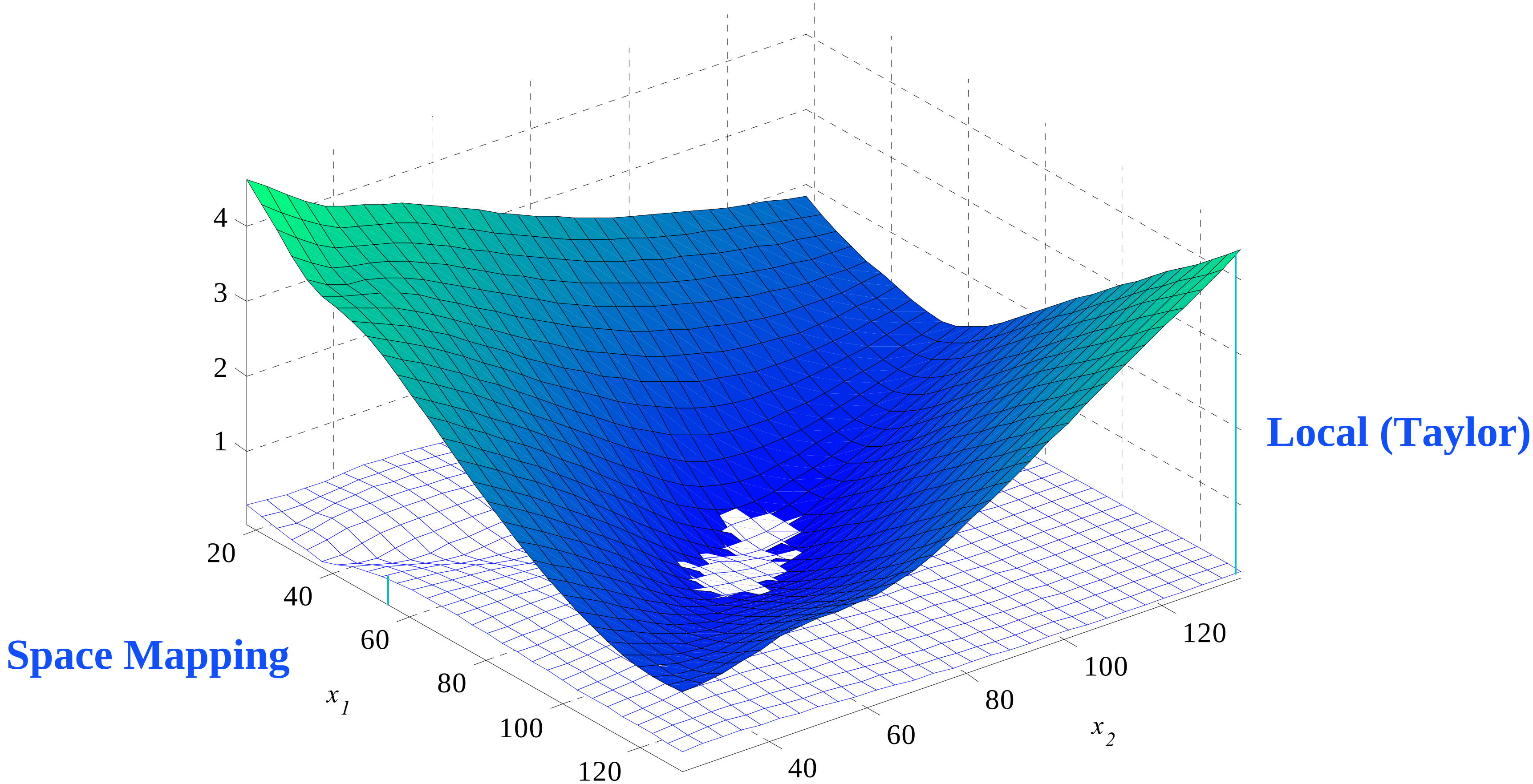
Taylor error at $x^{(i)}$

$$\left\| f(x) - f^{(i)}(x) \right\| \le C_T \cdot \left\| x - x^{(i)} \right\|^2$$

SM error at $x^{(i)}$

$$\left\| f(x) - c(P^{(i)}(x)) \right\| \le \varepsilon + \left\| J_c(P^{(i)}(x^{(i)})) \right\| \cdot C_{SM} \cdot \left\| x - x^{(i)} \right\|^2$$

Approximation Errors



Convergence Theory

Convergence has been proved for the combination of the Space Mapping with a traditional algorithm.

Vicente (2003), for the least squares objective.

Madsen, Søndergaard (2004), for a general objective.

i'th Surrogate Model

Assume P has been computed at $x^{(0)}, x^{(1)}, \ldots, x^{(i)}$

$$s_{SM}^{(i)}(x) \equiv c(B^{(i)}(x - x^{(i)}) + P(x^{(i)}))$$

Input Surrogate Model

(*Bandler et al., 1994*)

Surrogate: $s(x,p) \equiv c(Bx+d), \qquad p=(B,d)$

Assume f has been computed at $x^{(0)}, x^{(1)}, \ldots, x^{(i)}$

$$p^{(i)} \in \arg\min_{p} \left\{ \sum_{k=0}^{i} w_k \, \| f(x^{(k)}) - s(x^{(k)}, p) \| \right\}$$

$$s^{(i)}(x) \equiv s(x, p^{(i)})$$

$$x^{(i+1)} = \arg\min_{x} H(s^{(i)}(x))$$

Output Surrogate Model

(*Bandler et al., 2003*)

Surrogate: $s(x, p) \equiv A\,c(x) + b, \qquad p = (A, b)$

Assume f has been computed at $x^{(0)}, x^{(1)}, \ldots, x^{(i)}$

$$p^{(i)} \in \arg\min_{p} \left\{ \sum_{k=0}^{i} w_k \,\| f(x^{(k)}) - s(x^{(k)}, p) \| \right\}$$

$$s^{(i)}(x) \equiv s(x, p^{(i)})$$

$$x^{(i+1)} = \arg\min_{x} H(s^{(i)}(x))$$

(*John Dennis, private communication, 2002*)

Implicit Surrogate Model

(*Bandler et al., 2001*)

Surrogate: $s(x, x_p) \equiv c(x, x_p)$

Assume f has been computed at $x^{(0)}, x^{(1)}, \ldots, x^{(i)}$

$$x_p^{(i)} \in \arg\min_{x_p} \left\{ \sum_{k=0}^{i} w_k \, \| f(x^{(k)}) - s(x^{(k)}, x_p) \| \right\}$$

$$s^{(i)}(x) \equiv s(x, x_p^{(i)})$$

$$x^{(i+1)} = \arg\min_{x} H(s^{(i)}(x))$$

Output/Implicit Surrogate Model

Output SM surrogate (additive): $s(x,d) \equiv c(x) + d$

$$d^{(i)} \in \arg\min_{d} \left\{ \sum_{k=0}^{i} w_k \,\| f(x^{(k)}) - (c(x^{(k)}) + d) \| \right\}$$

Implicit SM surrogate: Let $s(x, x_p) = c(x) + x_p$

$$x_p^{(i)} \in \arg\min_{x_p} \left\{ \sum_{k=0}^{i} w_k \,\| f(x^{(k)}) - (c(x^{(k)}) + x_p) \| \right\}$$

Thus: Additive Output SM is a special case of Implicit SM

Input / Implicit Surrogate Model

Input SM surrogate: $s(x,p) \equiv c(Bx+d), \qquad p=(B,d)$

$$p^{(i)} \in \arg\min_{p} \left\{ \sum_{k=0}^{i} w_k \| f(x^{(k)}) - s(x^{(k)}, p) \| \right\}$$

Implicit SM surrogate:

$$s(x,x_p) \equiv c(Bx+d), \qquad x_p = (B,d)$$

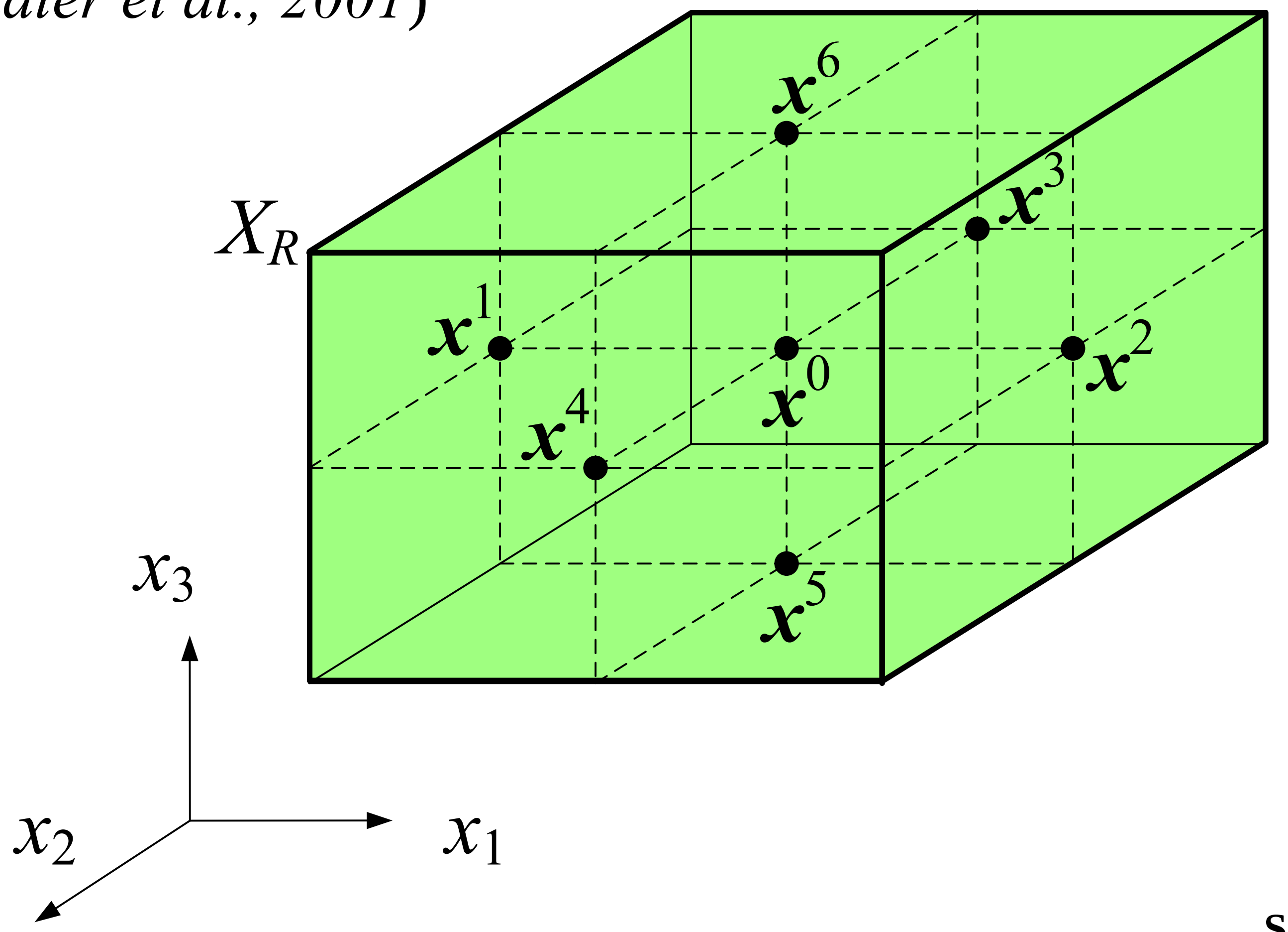
$$x_p^{(i)} \in \arg\min_{x_p} \left\{ \sum_{k=0}^{i} w_k \| f(x^{(k)}) - s(x^{(k)}, x_p) \| \right\}$$

Thus: Input SM can be considered a special case of Implicit SM

Space Mapping for Modelling

Star Distribution for SM-based Modelling

(*Bandler et al., 2001*)



Input/Output Surrogate Model

(*Bandler et al., 2003*)

Input surrogate: $s(x, B, d) \equiv c(Bx + d)$

Output surrogate: $s(x, A, b) \equiv Ac(x) + b$

Assume f has been computed at $x^{(0)}, x^{(1)}, \ldots, x^{(N)}$

$$(A^{(i)}, B^{(i)}, c^{(i)}, d^{(i)})$$

$$= \arg \min_{(A,B,c,d)} \left\{ \sum_{k=0}^{i} w_k \, \| f(x^{(k)}) - (A \cdot c(Bx^{(k)} + d) + b) \| \right\}$$

$$s^{(i)}(x_f) \equiv A^{(i)} c(B^{(i)} x + c^{(i)}) + d^{(i)}$$

Space Mapping-based Modelling

$$x \in X_R \equiv [\, x_{mid} - \delta, x_{mid} + \delta \,], \qquad \delta = [\delta_1, \delta_2, \ldots\ , \delta_N\,]$$

$$(A^{(i)}, B^{(i)}, b^{(i)}, d^{(i)})$$
$$= \arg \min_{(A,B,b,d)} \left\{ \sum_{k=0}^{N} w_k \,\|\, f(x^{(k)}) - (A \cdot c(B\,x^{(k)} + d) + b) \,\|\, \right\}$$

$$s^{(i)}(x) \equiv \; A^{(i)} c(B^{(i)} x + d^{(i)}) + b^{(i)}$$

$$w_k \equiv w_k(x, C, \lambda) = \frac{\exp\left(- \dfrac{\| x - x^{(k)} \|^2}{C\lambda^2} \right)}{\sum\limits_{j=1}^{N} \exp\left(- \dfrac{\| x - x^{(j)} \|^2}{C\lambda^2} \right)} \qquad \lambda = \frac{2}{n \cdot N^{1/n}} \sum_{i=1}^{n} \delta_i$$

The SM based modelling technique is arbitrarily accurate:

Theorem

Let $X_B \equiv \{x^{(0)}, x^{(1)}, \ldots, x^{(N)}\}$.

Suppose certain regularity conditions are satisfied.

Let $\varepsilon > 0$ be given. Then there exists $\eta > 0$ such that:

If $\forall x \in X_R \quad \exists x^{(k)} \in X_B : \| x - x^{(k)} \| < \eta$

then $\| f(x) - s(x) \| < \varepsilon$ for any $x \in X_R$

provided C > 0 is sufficiently small.

Koziel, Bandler, Madsen (2006)

Convergence Theory

Convergence of the different variations of the Space Mapping has been proved under certain regularity and Lipschitz conditions.

(*Koziel, Bandler, Madsen* (*2005*))

(*Koziel's talk at 16.45 tomorrow*)

Conclusions

- Space Mapping provides powerful surrogate models (mapped coarse models) applicable in optimization as well as in modelling
- Space Mapping has been successfully applied to numerous engineering problems
- The Input SM, Output SM, and Implicit SM Space Mapping algorithms originate from engineering practice. They are similar in theory, however they perform differently in practice
- Space Mapping is provably convergent
- Space Mapping requires skilled engineers for designing the coarse models