On Useful Redundancy in Dynamic Inverse Problem Related Optimization

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(Work supported by the French ANR-CLPP)

Chemical and Biological Processes

- Highly nonlinear dynamic
- Badly known parameters
- Lack of sensors

$\rightarrow$ Need for nonlinear observers

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Analytic nonlinear observers

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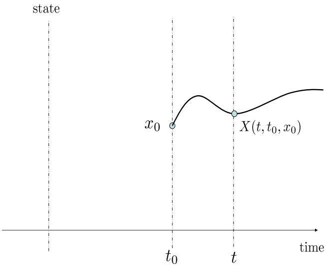

$$x(t) = X(t, t_0, x_0)$$
$$y = h(x)$$

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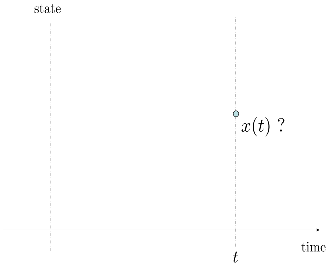

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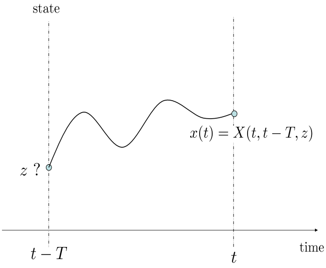

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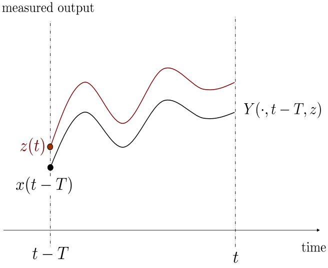

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$$x(t) = X(t, t_0, x_0)$$
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$$z_{opt}(t) \leftarrow arg \min_z \quad J_0(z, t, y_{t-T}^t) = \int_{t-T}^t \|Y(\tau, t-T, z) - y(\tau)\|_Q^2 d\tau$$

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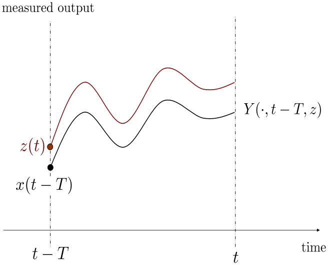

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$$\hat{x}(t) := X(t, t-T, z_{opt}(t))$$

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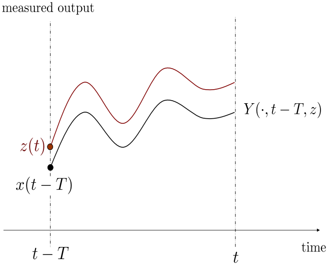

- *Generally a non convex optimization problem*
- *many local minima*

$$z_{opt}(t) \leftarrow arg \min_z \quad J_0(z, t, y_{t-T}^t) = \int_{t-T}^t \|Y(\tau, t-T, z) - y(\tau)\|_Q^2 d\tau$$

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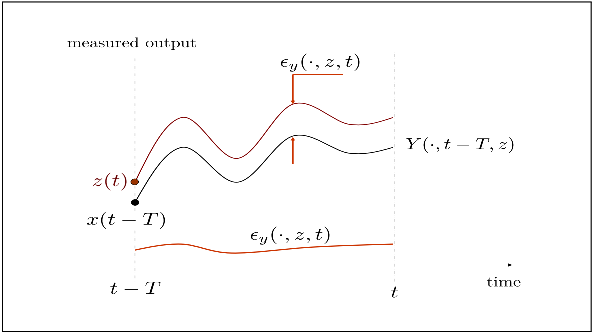
A very particular problem . . . !



$$z_{opt}(t) \leftarrow arg \min_{z} \quad J_0(z, t, y_{t-T}^{t}) = \int_{t-T}^{t} \| Y(\tau, t-T, z) - y(\tau) \|_Q^2 d\tau$$

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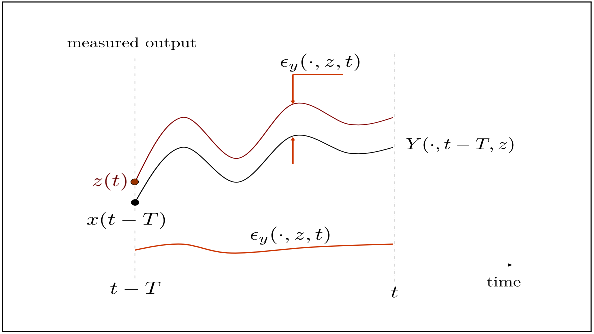

$$z_{opt}(t) \leftarrow arg \min_{z} \quad J_0(z, t, y_{t-T}^t) = \int_{t-T}^{t} \|\epsilon_y(\tau, z, t)\|_Q^2 d\tau$$

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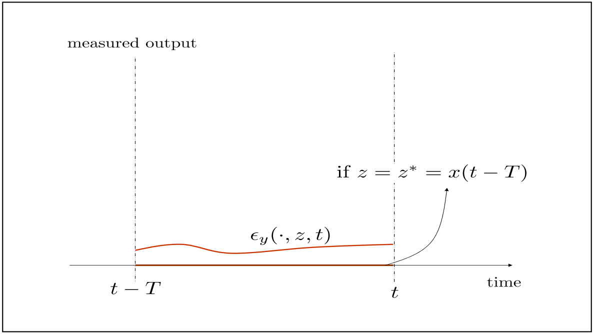

$$z_{opt}(t) \leftarrow arg \min_z \quad J_0(z, t, y_{t-T}^t) = \int_{t-T}^t \|\epsilon_y(\tau, z^*, t)\|_Q^2 d\tau = 0$$

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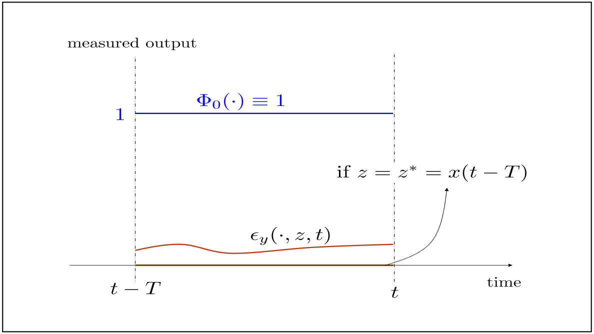

$$z_{opt}(t) \leftarrow arg \min_{z} \quad J_0(z, t, y_{t-T}^t) = \int_{t-T}^{t} \Phi_0(\tau) \cdot \|\epsilon_y(\tau, z^*, t)\|_Q^2 d\tau = 0$$

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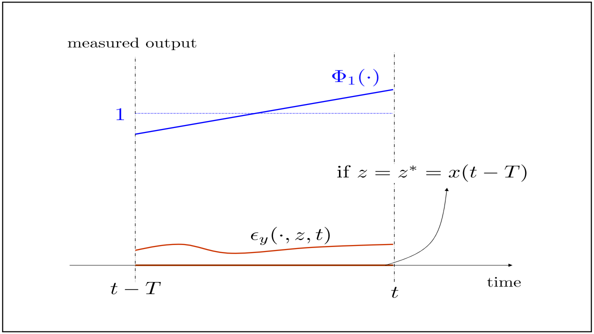
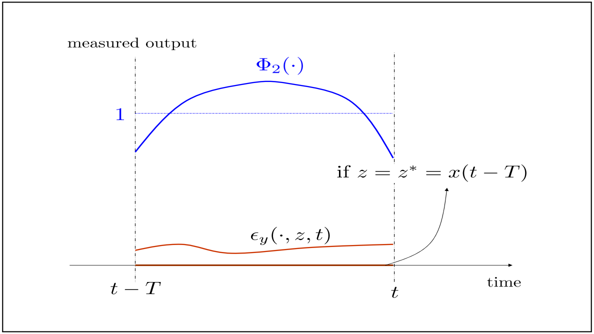


$$z_{opt}(t) \leftarrow arg \min_z \quad J_1(z, t, y_{t-T}^t) = \int_{t-T}^t \Phi_1(\tau) \cdot \|\epsilon_y(\tau, z^*, t)\|_Q^2 d\tau = 0$$

A very particular problem . . . !



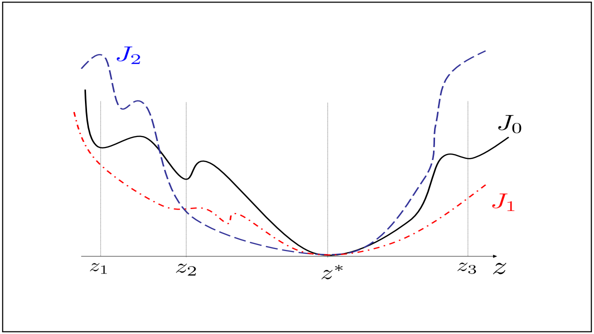
$$z_{opt}(t) \leftarrow arg \min_z \quad J_2(z, t, y_{t-T}^t) = \int_{t-T}^t \Phi_2(\tau) \cdot \|\epsilon_y(\tau, z^*, t)\|_Q^2 d\tau = 0$$

A very particular problem . . . !

z^* is THE global minimum of ALL the cost functions J_i s.t:

$$J_i(z, t, y_{t-T}^{t}) = \int_{t-T}^{t} \Phi_i(\tau) \cdot \Psi\big(\epsilon(\tau, z, t)\big)\, d\tau$$

A very particular problem . . . !



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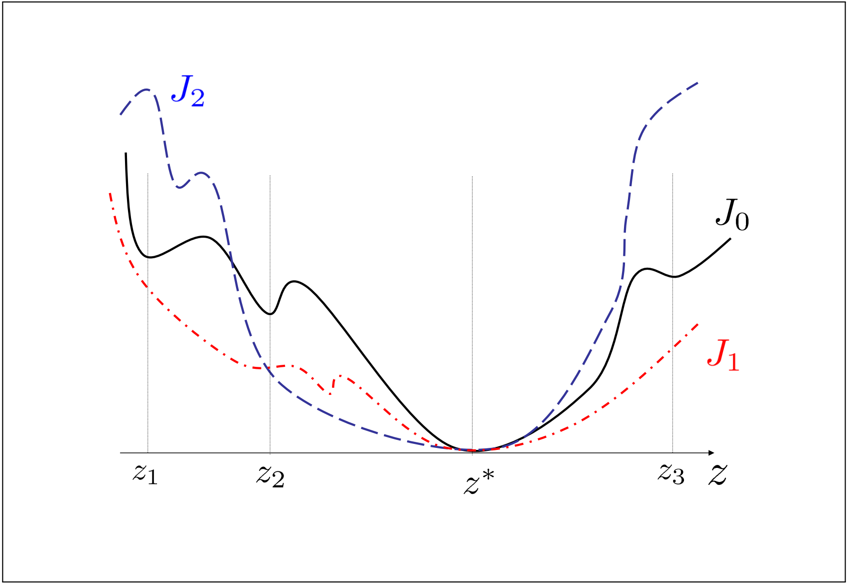
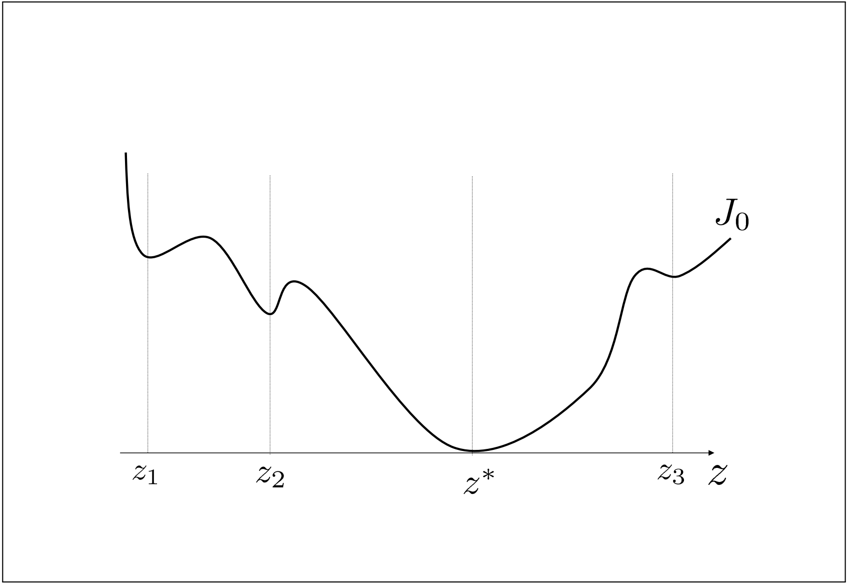
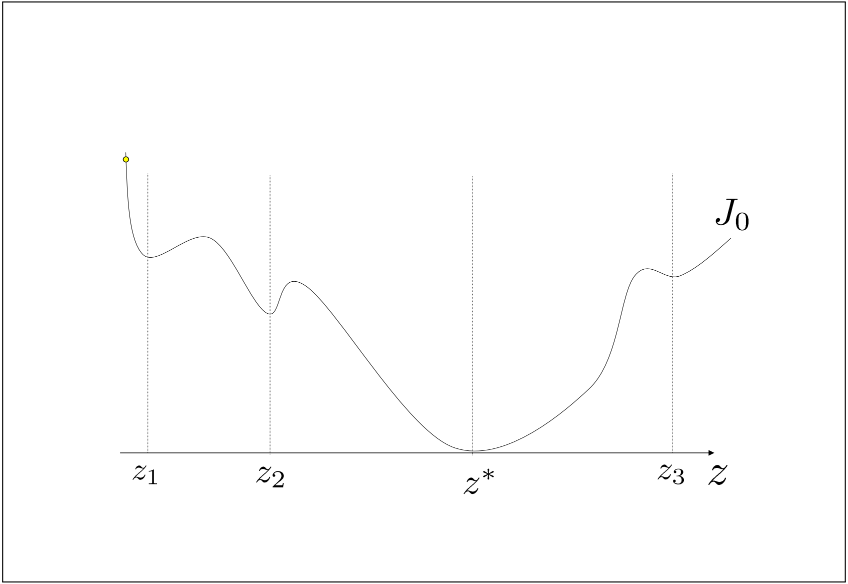

J_2
J_0
J_1
z_1
z_2
z^*
z_3
z


J_0
z_1
z_2
z^*
z_3
z


J_0
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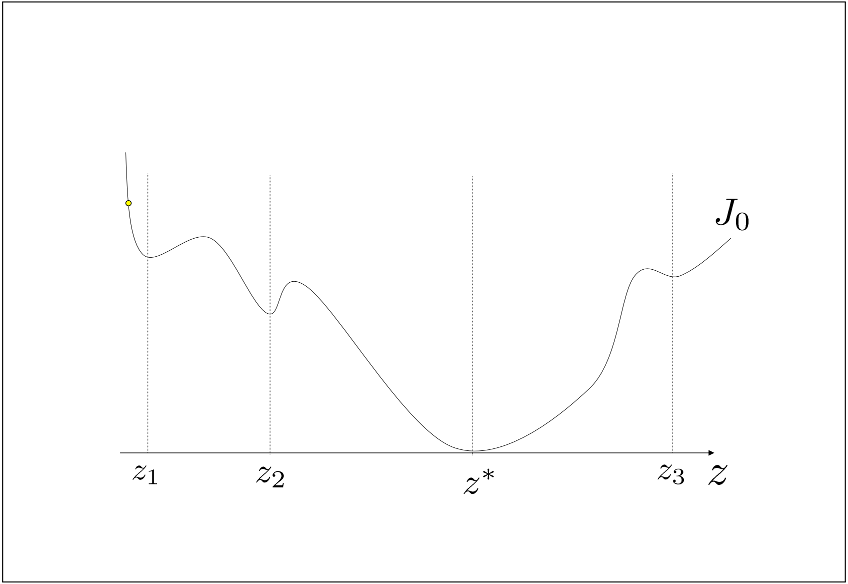
J_0
z_1
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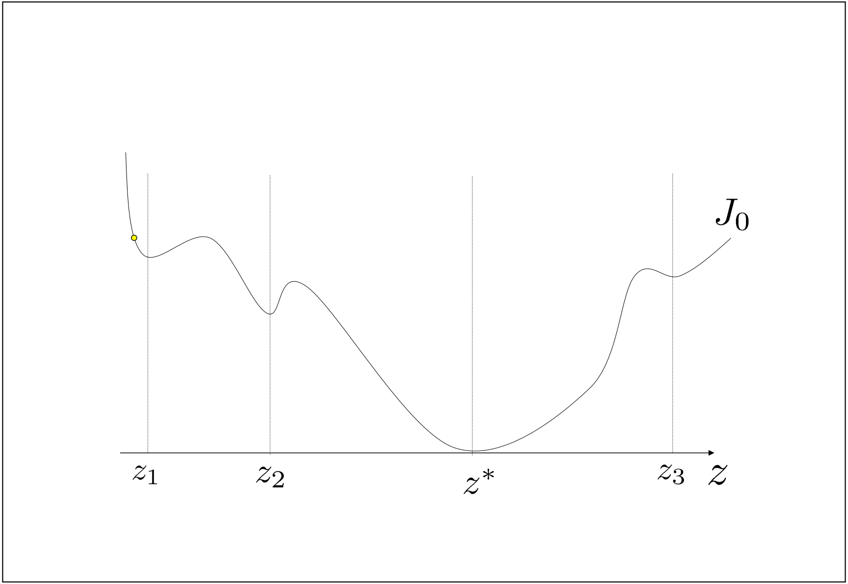
z_3
z


J_0
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z_3
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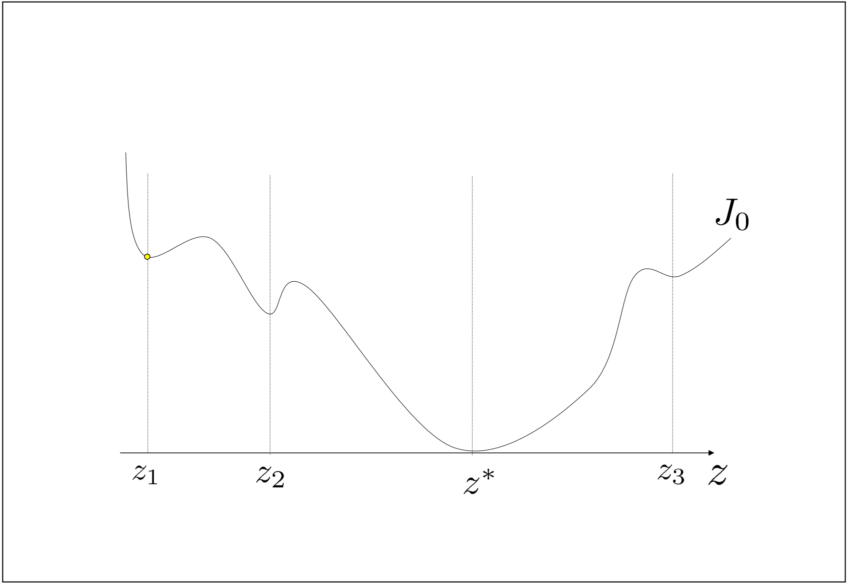
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z_2
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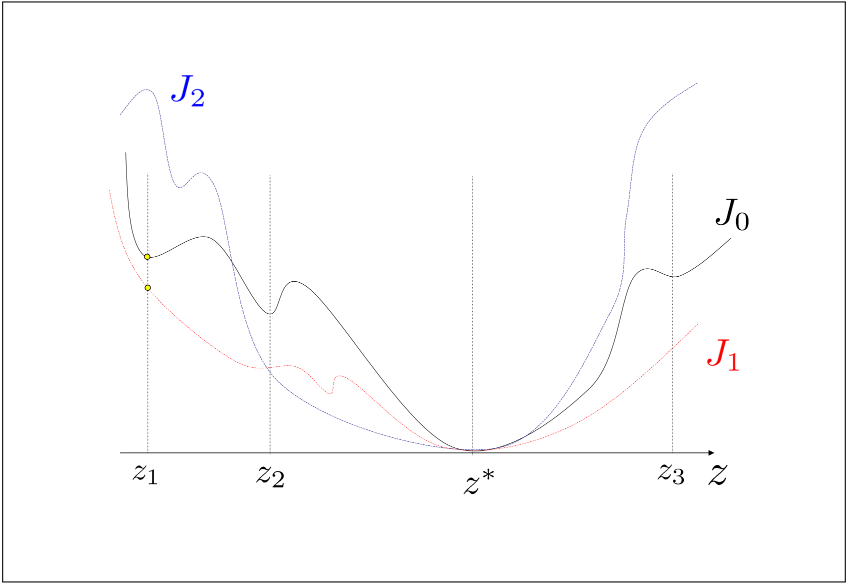

J_2
J_0
J_1
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z_3
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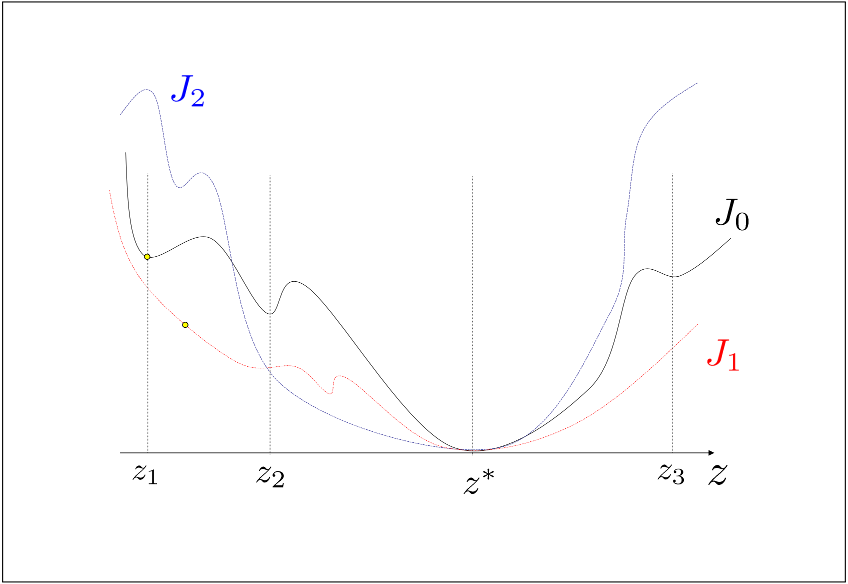
J_2
J_0
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z_1
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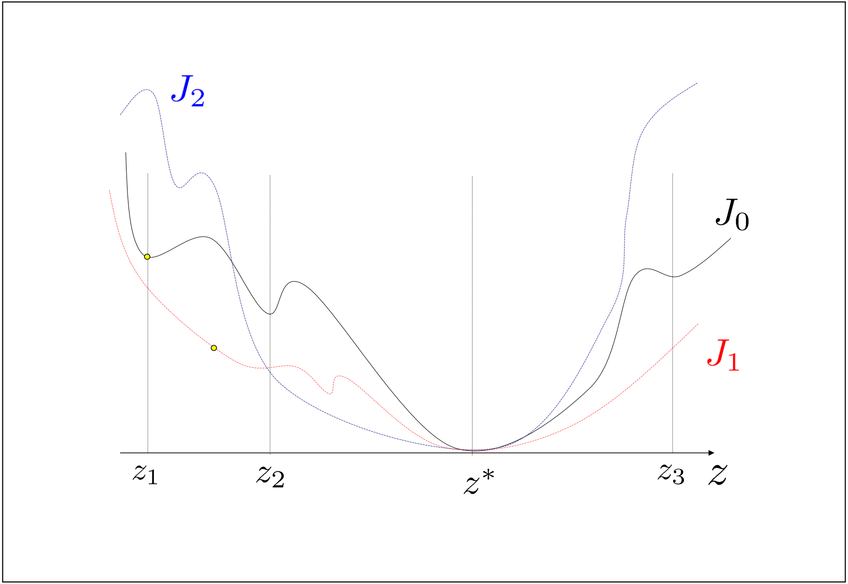
z_3
z


J_2
J_0
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z^*
z_3
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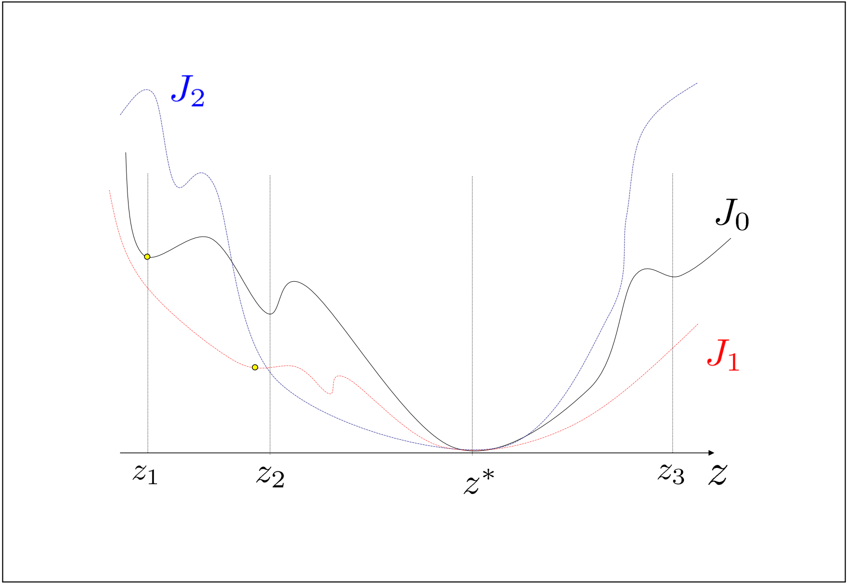
J_2
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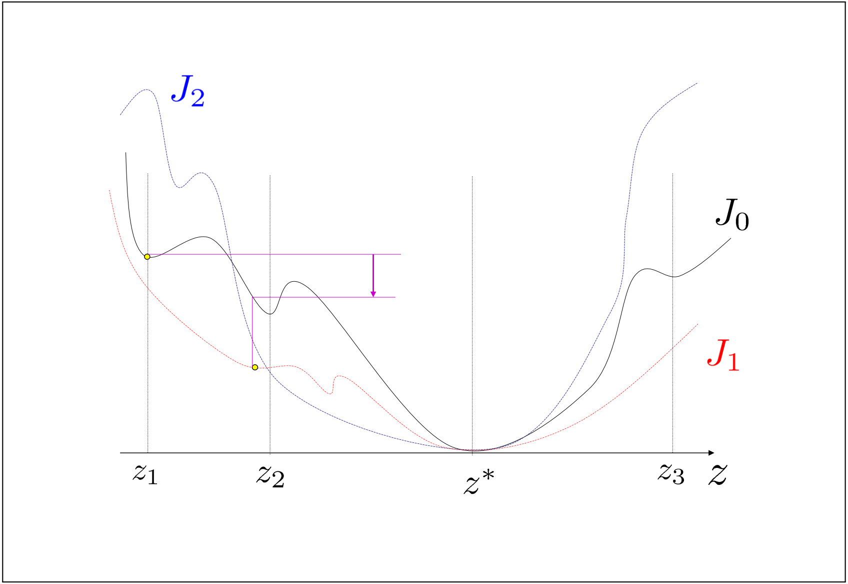

J_2
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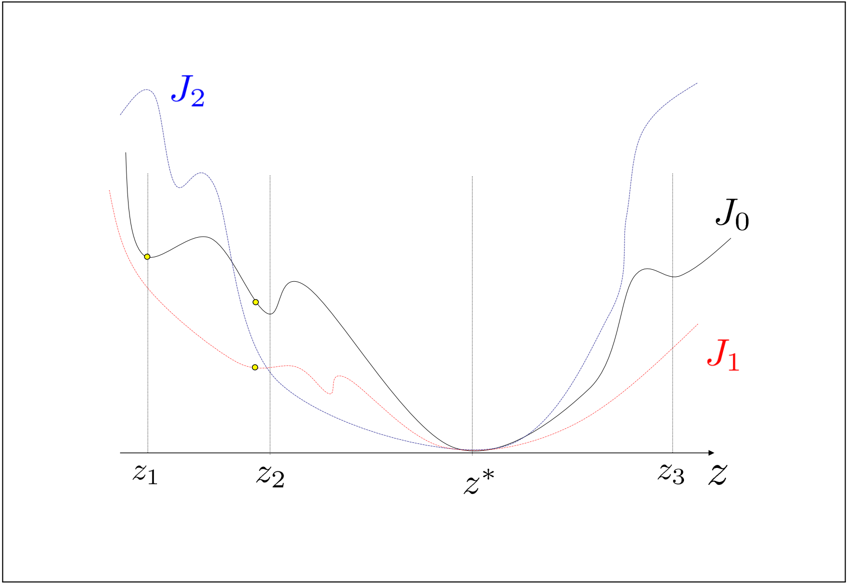
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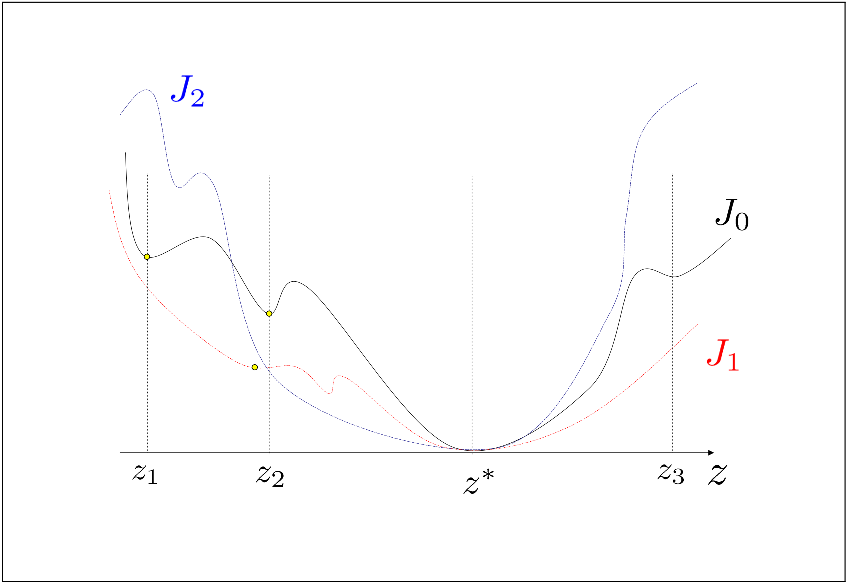
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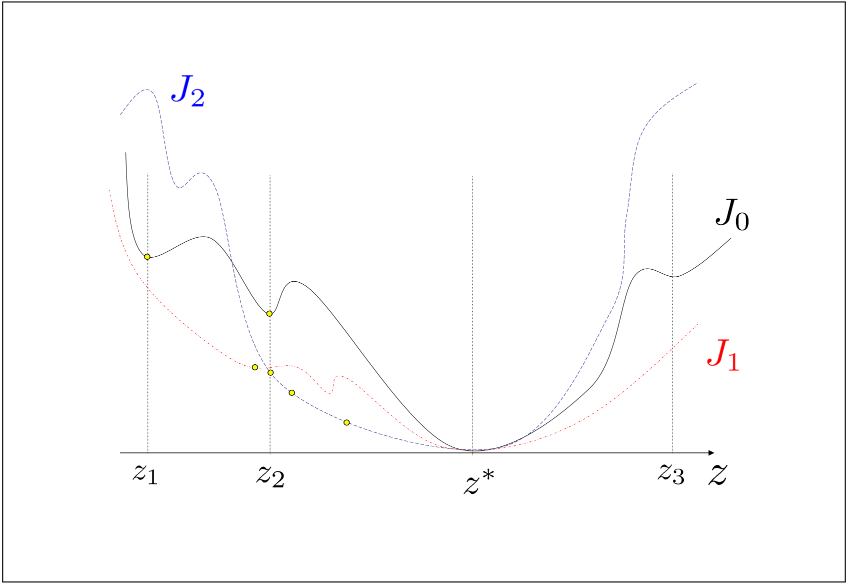

J_2
J_0
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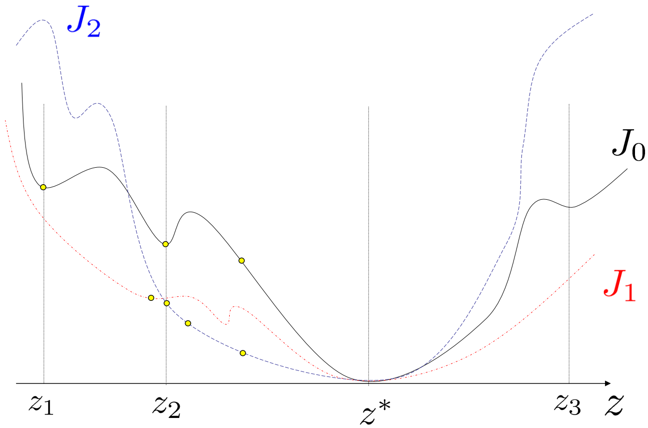
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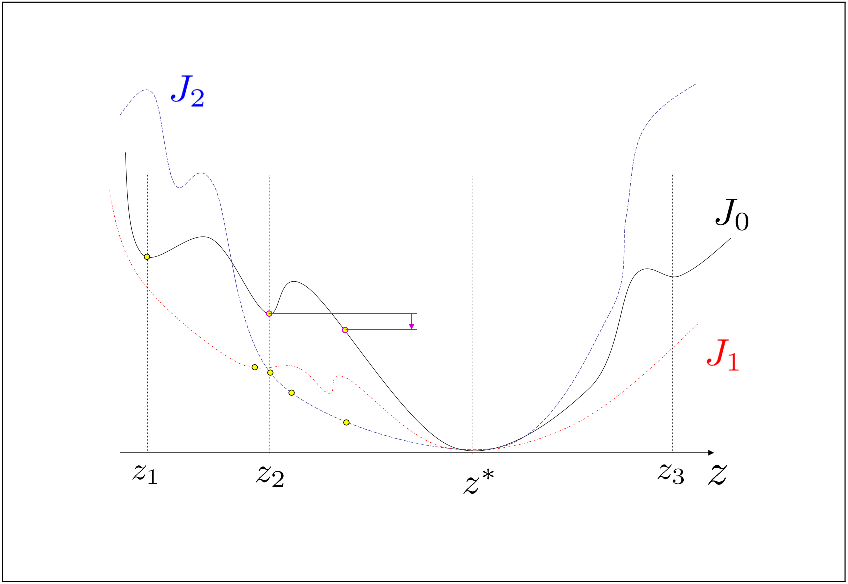
J_2
J_0
J_1
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z_2
z^*
z_3
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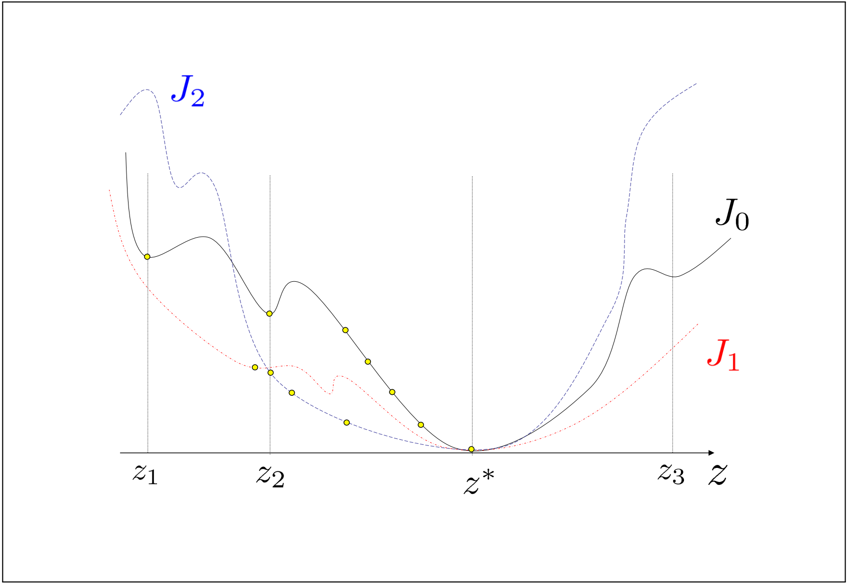
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J_0
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z^*
z_3
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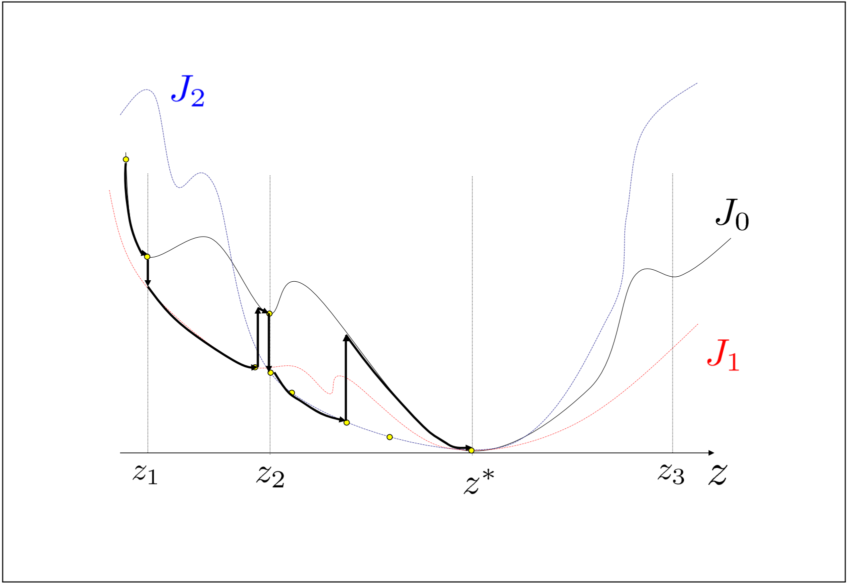
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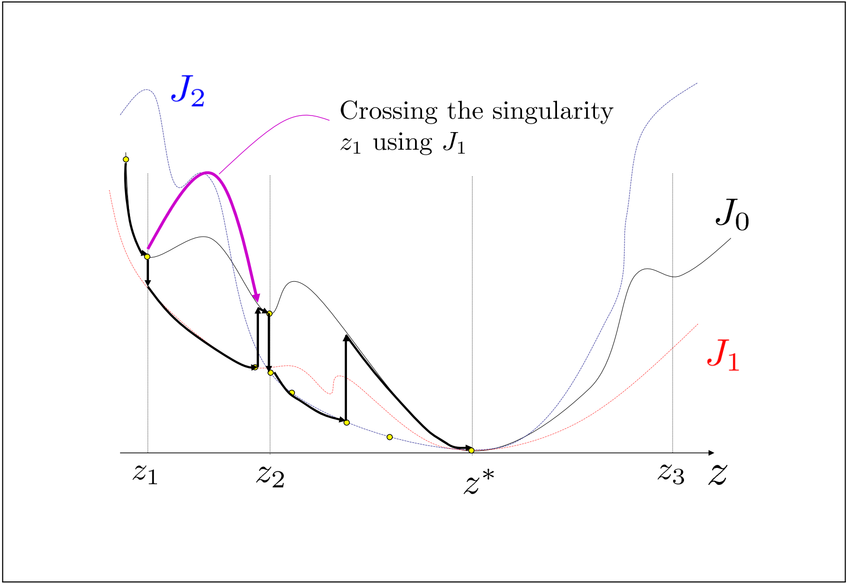
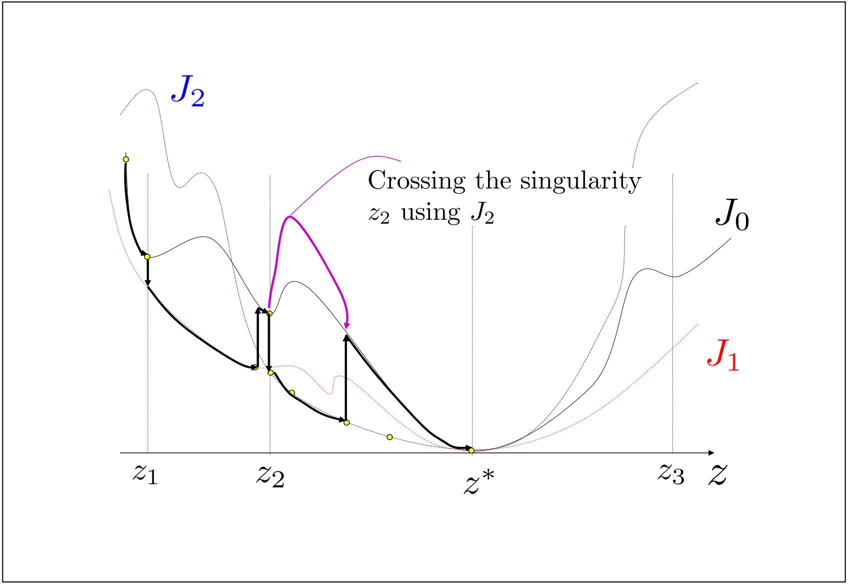
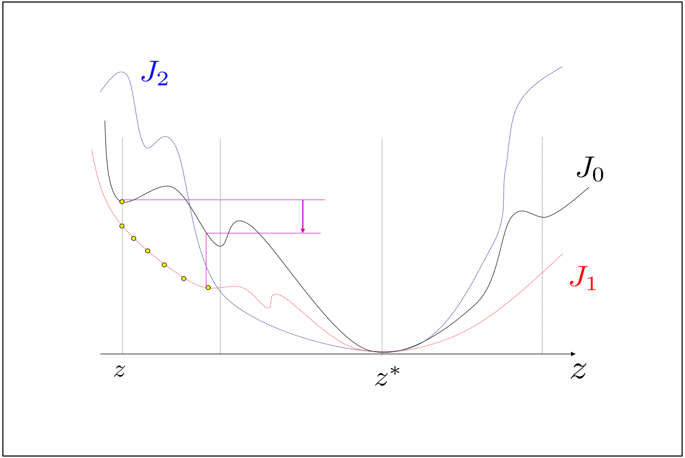
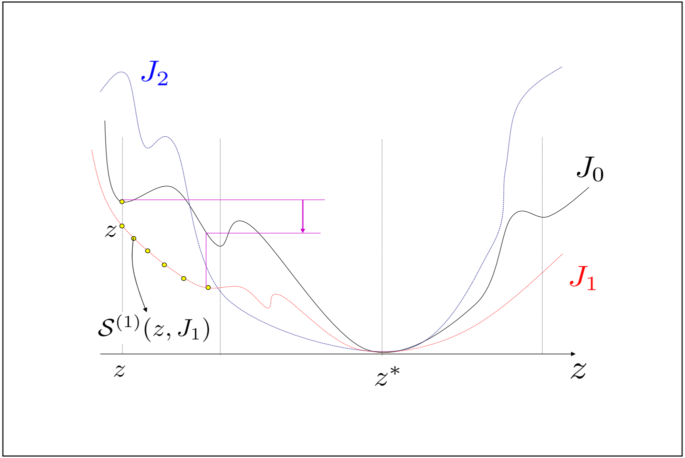
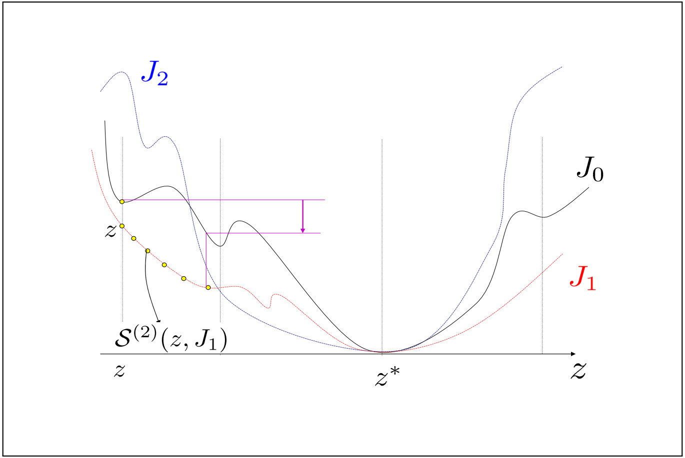


J2
Crossing the singularity
z1 using J1
J0
J1
z1
z2
z*
z3
Z

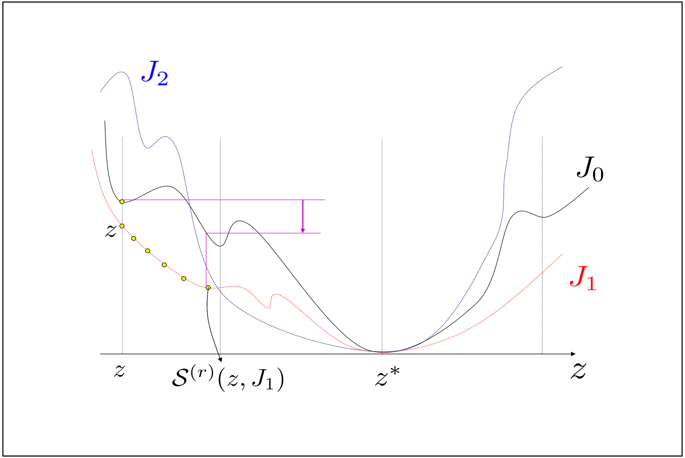

J_2
Crossing the singularity
z_2 using J_2
J_0
J_1
z_1
z_2
z^*
z_3
z


J_2
J_0
J_1
z
z^*
Z

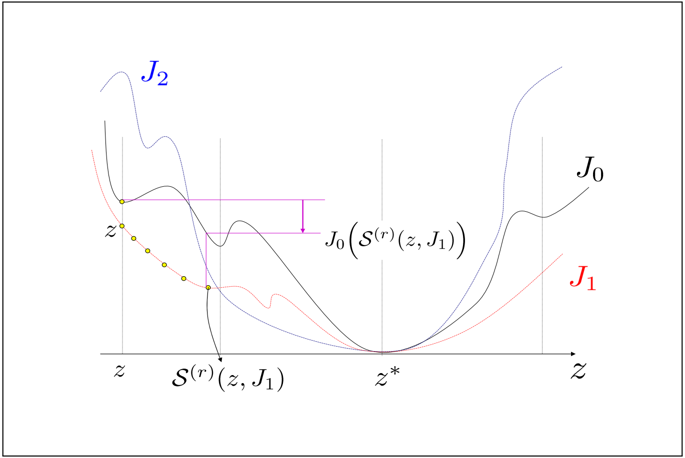

J_2
J_0
J_1
z
$\mathcal{S}^{(1)}(z, J_1)$
z
z^*
Z

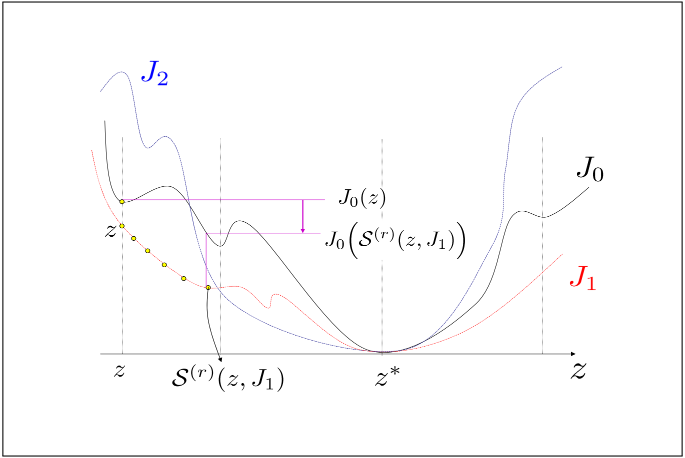


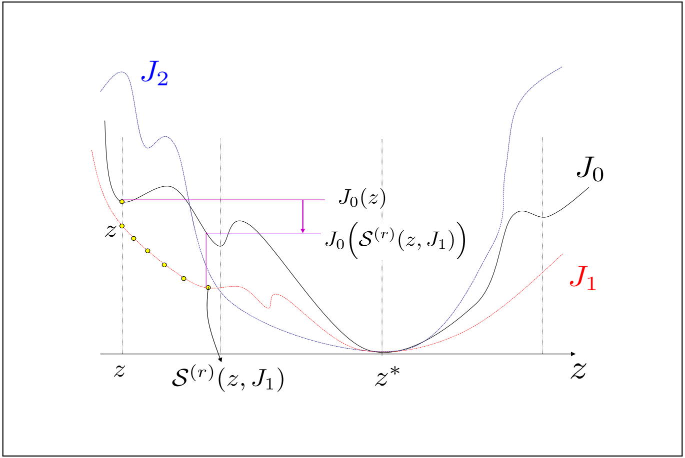
J_2
J_0
J_1
z
$\mathcal{S}^{(2)}(z, J_1)$
z
z^*
$\mathcal{Z}$



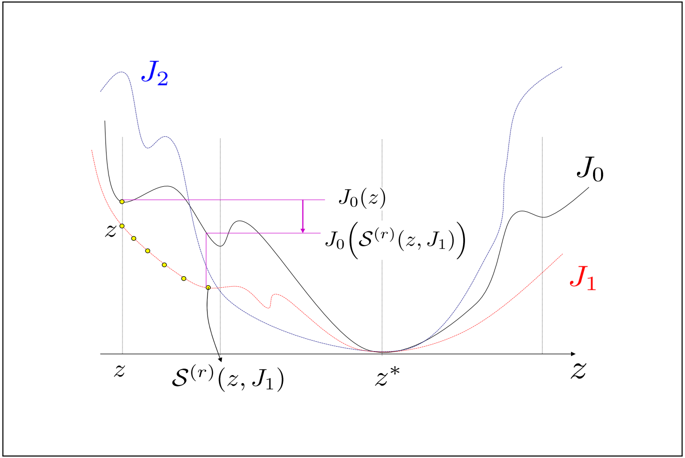
J_2
J_0
J_1
z
z
$\mathcal{S}^{(r)}(z, J_1)$
z^*
$\mathcal{Z}$


J_2
J_0
$J_0\left(\mathcal{S}^{(r)}(z, J_1)\right)$
J_1
z
z
$\mathcal{S}^{(r)}(z, J_1)$
z^*
$\mathcal{Z}$


J_2
J_0
$J_0(z)$
$J_0\Big(\mathcal{S}^{(r)}(z, J_1)\Big)$
z
J_1
z
$\mathcal{S}^{(r)}(z, J_1)$
z^*
Z



$$\Delta(z) := \min_{i \in \{0,\dots,N\}} \left[J_0(\mathcal{S}^{(r^*)}(z, J_i)) - \gamma J_0(z) \right] \leq 0$$



$$(\exists r^*)\ (\forall z) \quad \Delta(z) := \min_{i\in\{0,\dots,N\}} \Big[J_0(\mathcal{S}^{(r^*)}(z, J_i)) - \gamma J_0(z) \Big] \leq 0$$

In the paper

- Precise formulation
- Dedicated algorithm
- Parallel computing version

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Hereafter

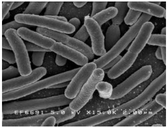
- Bio-reactor State estimation example
- Parameter estimation example / comparison:
  - Multiple starting points
  - Redundancy-Based singularity avoidance

Example 1: Recombinant Escherichia Coli

$$\dot{X} = \mu(S)X - k_d \exp(-\frac{k_p}{P})X$$
$$\dot{S} = -y_s\mu X - k_m X$$
$$\dot{P} = y_p\mu(S)\frac{I}{I+k_I}X - k_d \exp(-\frac{k_p}{P})P$$

- X: *E. Coli* strain
- S: substrate glycerol
- P: intracellular product β-galactosidase protein
- μ is the growth rate

$$\mu(S) = \frac{\mu_m S}{k_s + S}$$

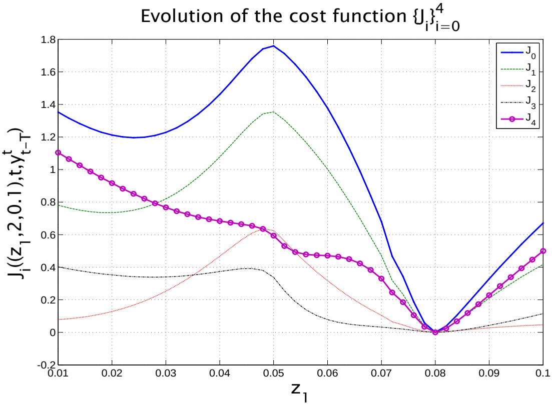


Escherichia coli under 15000 magnification factor

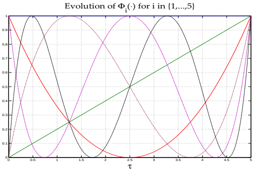
Output measurement:

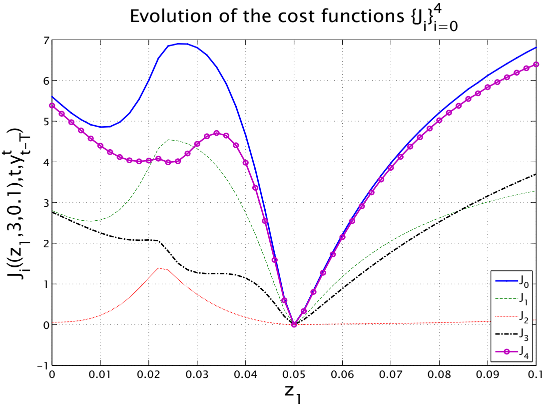
Light produced by the bioluminescence:

$$L = y_l \cdot \mu(S)\frac{I}{I+k_I}XP$$

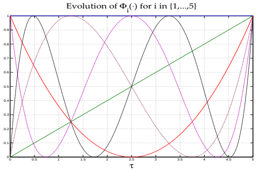


- $T = 10$
- $x(t - T) = (0.08, 2, 0.1)$
- $z_2 = x_2(t - T)$, $z_3 = x_3(t - T)$





- $T = 15$
- $x(t-T) = (0.05, 3, 0.1)$
- $z_2 = x_2(t-T)$, $z_3 = x_3(t-T)$



Example 2: Parameter estimation

$$
\begin{aligned}
\dot{x}_1 &= -p_1 x_2 \\
\dot{x}_2 &= (1+p_2)x_1 + (1-x_1^2)x_2 \\
y &= x_1 + x_2 + \nu
\end{aligned}
$$

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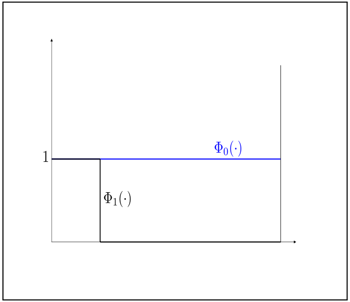
$$\dot{x}_2 = (1+p_2)x_1 + (1-x_1^2)x_2$$
$$y = x_1 + x_2 + \nu$$



Example 2: Parameter estimation

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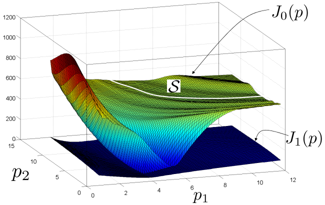

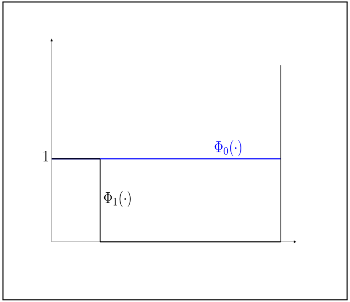

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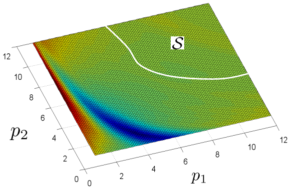

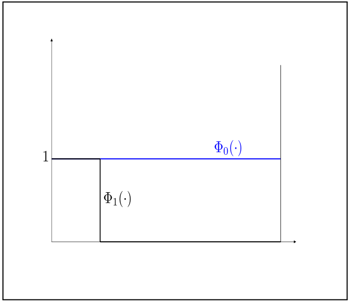

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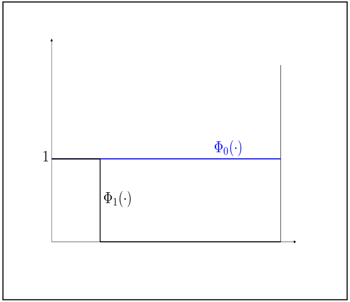

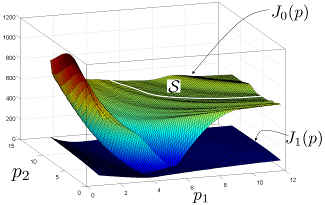

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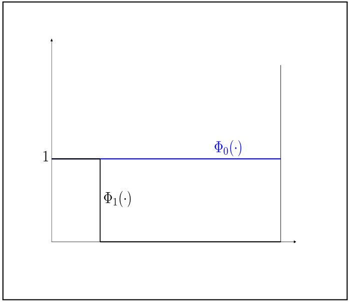

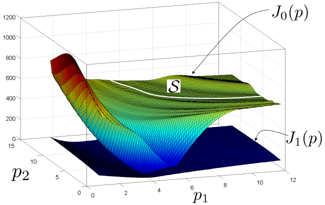

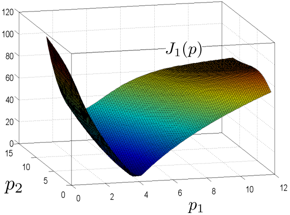

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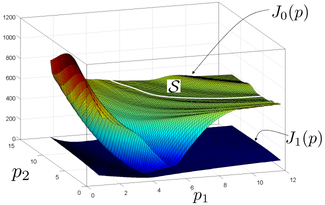

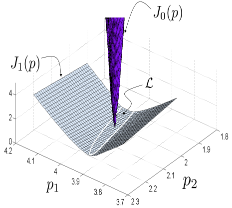

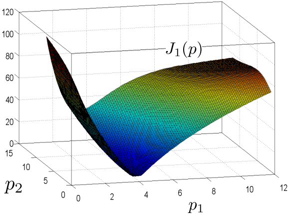

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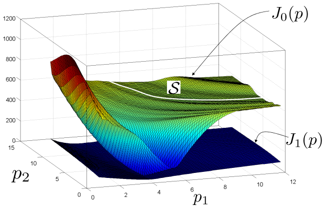
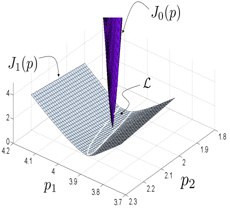
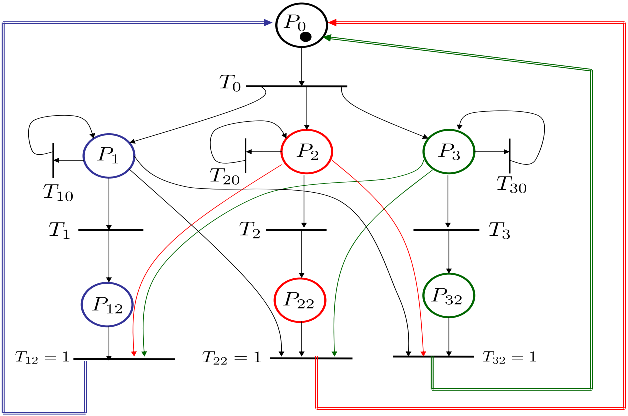




i	Algorithm 1	Algorithm 2
1	$Pr\left[J_0(p^{(m,i)}) > 400\right] \geq 0.25$	Conv. to $\mathcal{L}$
2	$Pr\left[J_0(p^{(m,i)}) > 400\right] \geq (0.25)^2$	Conv. to $\{p^r\}$
3	$Pr\left[J_0(p^{(m,i)}) > 400\right] \geq (0.25)^3$	Conv. to $\{p^r\}$
⋮	⋮	⋮

Conclusion

- Dynamic inversion leads to particular optimization problems
- Singularity crossing algorithm based on redundancy
- $\neq$ multiple starting points
- Scheme that is solver-independent
- Additional *layer* to any existing *global* scheme


P_0
T_0
P_1
P_2
P_3
T_{10}
T_{20}
T_{30}
T_1
T_2
T_3
P_{12}
P_{22}
P_{32}
$T_{12} = 1$
$T_{22} = 1$
$T_{32} = 1$

$$x^+ = f(x, u, p)$$
$$y = h(x, p) + w$$

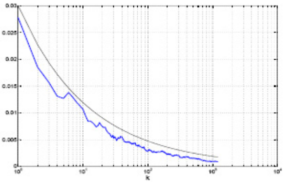
- $u_k = \mathcal{U}(k, q)$ with $q \in \mathbb{Q}$
- $y_k^0(q, p)$ prediction under $w \equiv 0$
- y_k^m effective measurement
- p^r true value of p
- $\epsilon_k(q, p^r, p) = y_k^0(q, p) - y_k^0(q, p^r)$

$$d^+(w, w^*) := \max\left\{0, |w| - w^*\right\}$$

(component wise)

Assumption on measurement errors w

$$\frac{\sum_{i=0}^{k^*-1} w(k+i)}{k^*} \in \phi_w(k^* - 1) \cdot [-\bar{w}, \bar{w}]$$



The l.h.s of the equation beside for for a MATLAB's $0.01 \times$ RANDN function (maximum over 1000 trials) and its approximated upper bound $\bar{w} \cdot \phi_w(k) = 0.03/(k^{0.4})$

gipsa-lab