Multi-period Sequential Synthesis of Heat Exchanger Networks with selection, design and operation of Multiple Utilities

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Outline

1. Introduction
2. Problem Statement
3. Sequential vs Simultaneous Approaches and solving strategies
5. Test Case and Results
   5.1 Literature Case
6. Conclusion
Challenges in Chemical and Power plant design:

1) Need of selecting among several technologies – superstructure approach

2) Integration of thermal/mass storage;

3) Schedule plant operations;

4) Minimize Total Yearly Costs;

Application to industry:

• Continuous processes
• Batch processes
• hybrid plants accounting for renewables
2. Problem Statement

*Given:*  
• a set of hot and cold process streams with given time dependent mass flow rates, time dependent inlet and outlet temperatures,  
• a set of available utility systems (e.g., cooling water, boiler, multiple-level steam cycle, refrigeration cycle, heat pump, etc) with fixed temperature levels, given superstructure of possible configurations and given part-load performance maps (relating efficiency to load)  
• optional heat/energy storage systems,  
• cost data relative to heat exchangers and utility systems,  

*Determine:*  
• the optimal selection, size and load in each period of the utility systems, such as Total Yearly Costs are minimized  
• the optimum heat exchanger network configuration as well as design.
2. Problem statement

Example of Objective Function

Objective function:
- not continuous
- not derivable
- vertical jumps activated by integer variables: e.g. selection of utility units and matches between hot and cold process/utility thermal and electricity streams
2. Sequential vs Simultaneous approaches

Sequential Approach (Floudas Superstructure)

Advantages:
- Capability to treat problems with higher number of streams;
- Superstructure with non-isothermal mixing allowed

Disadvantages:
- Optimization constraints are non-linear (Mixers-LMTD)
- Sequential does not allow to properly estimate trade-offs between utilities, Nex, Aex
2. Sequential vs Simultaneous approaches
2. Sequential vs Simultaneous approaches

Simultaneous Approach (SYNHEAT Superstructure):

Advantages:

- All optimization constraints are linear, only linearity in objective function

- Simultaneous resolution allows to correctly estimate trade-offs between utilities, Nex, Aex

Disadvantages:

- only isothermal mixing is possible

- suitable for small problems

- HU and CU only at top and bottom of Hottest/Coldest process streams

- Demonstrated to be NP-Hard Programming Problem
2. Sequential vs Simultaneous approaches
\[
\begin{align*}
\text{min} & \quad \sum_i \sum_j \sum_k c_f z_{ijk} + \sum_i \sum_j c_f z_{cu} + \sum_i \sum_j c_{cu} q_{cu} + \sum_j c_{hu} q_{hu} \quad \Rightarrow \quad \text{Minimum total annual cost SYNHEAT Model} \\
\sum_i \sum_j \sum_k c \left( \frac{q_{ijk}}{U_{ij} LMTD_{ijk}} \right)^{\beta} + \sum_i c \left( \frac{q_{cu}}{U_{cu} LMTD_{cu} i} \right)^{\beta} + \sum_j c \left( \frac{q_{hu}}{U_{hu} LMTD_{hu} j} \right)^{\beta} \\
\text{subject to} & \quad \sum_i \sum_j \sum_k q_{ijk} + q_{cu} = F_i \left( T_{i}^{in} - T_{i}^{out} \right), i \in HP \\
& \quad \sum_j \sum_k q_{ijk} + q_{hu} = F_j \left( T_{j}^{out} - T_{j}^{in} \right), j \in CP \\
& \quad \sum_j q_{ijk} = F_i \left( t_{i}^{k} - t_{i}^{k+1} \right), i \in HP \\
& \quad \sum_j q_{ijk} = F_j \left( t_{j}^{k} - t_{j}^{k+1} \right), j \in CP \\
& \quad t_{i}^{k=1} = T_{i}^{in} , t_{j}^{k=NOK} = T_{j}^{in} \\
& \quad t_{i}^{k} \geq t_{i}^{k+1} , t_{j}^{k} \geq t_{j}^{k+1} \\
& \quad t_{i}^{k=NOK+1} \geq T_{j}^{out} , t_{j}^{k=NOK} \geq T_{j}^{out} \\
& \quad q_{cu} = F_i \left( T_{i}^{NOK+1} - T_{i}^{out} \right) \\
& \quad q_{hu} = F_j \left( T_{j}^{out} - T_{j}^{in} \right) \\
& \quad dt_{ijk} \geq \Delta T_{min}, dt_{cu} \geq \Delta T_{min}, dt_{hu} \geq \Delta T_{min} \\
& \quad q_{ijk} \geq \Omega z_{ijk}, q_{cu} \geq \Omega z_{cu}, q_{hu} \geq \Omega z_{hu} \\
& \quad dt_{ijk} \geq t_{i}^{k} - t_{j}^{k+1} + \Gamma \left( 1 - z_{ijk} \right) \\
& \quad dt_{ijk} \geq t_{i}^{k+1} - t_{j}^{k+1} + \Gamma \left( 1 - z_{ijk} \right) \\
& \quad dt_{cu} \geq t_{i}^{NOK} - t_{j}^{cu} + \Gamma \left( 1 - z_{cu} \right) \\
& \quad dt_{cu} \geq T_{i}^{cu} - t_{j}^{cu} + \Gamma \left( 1 - z_{cu} \right) \\
& \quad dt_{hu} \geq t_{i}^{out} - t_{j}^{hu} + \Gamma \left( 1 - z_{hu} \right) \\
& \quad dt_{hu} \geq t_{i}^{out} - t_{j}^{hu} + \Gamma \left( 1 - z_{hu} \right) \\
& \quad LMTD_{ijk} = \frac{dt_{ijk} - dt_{ijk+1}}{\ln \left( \frac{dt_{ijk}}{dt_{ijk+1}} \right)} \\
& \quad LMTD_{cu} = \frac{dt_{ijk} - dt_{cu}}{\ln \left( \frac{dt_{ijk}}{dt_{cu}} \right)} , LMTD_{hu} = \frac{dt_{ijk} - dt_{hu}}{\ln \left( \frac{dt_{ijk}}{dt_{hu}} \right)} \\
& \quad T_{i}^{out} \leq t_{i}^{k} \leq T_{i}^{in} , \quad T_{j}^{in} \leq t_{j}^{k} \leq T_{j}^{out} \\
& \quad q_{ijk} , q_{cu} , q_{hu} \geq 0 \quad \text{Nonnegativity constraints} \\
& \quad z_{ijk} , z_{cu} , z_{hu} = 0 \quad \text{Integrality conditions} \\
\end{align*}
\]
2. Solving Strategies for Sequential/Simultaneous approaches

Derivative Based vs Derivative Free

Derivative Based:
- Need of a feasible starting point
- Sensible to degree of non convexity of the problem
- Convergence is not guaranteed for discontinuous Objective Functions (OF)

Derivative Free:
- Need of enough OF evaluations for the convergence
- Not sensible to degree of non-convexity of the problem
- Can handle discontinuous and not derivable objective functions
\[
\min_{x_t \in \Omega_t} \{ f_t(x_t) \} \\
\]
\[
x_t = \left\{ \begin{array}{l}
y_u^t, f_u^t \\
y_{u, fu}^t, f_{u, fu}^t \\
R^t_k \\
\end{array} \right\}
\]
\[
\begin{align*}
\sum_{u=1}^{n_u} f_{u, k}^t \cdot q_{u, k} + \sum_{s=1}^{n_s} Q_{s, k} + R^t_k - R^t_{k-1} &= 0 & \text{heat balance of temperature intervals} \\
R^t_k &= 0 & \forall \, t = 1, \ldots, N, k = 1, \ldots, n_{k-1} \\
R^t_k &\geq 0 & \forall \, t = 1, \ldots, T, k = 1, \ldots, n_{k-1} \\
\sum_{u=1}^{n_u} f_{u, k}^t \cdot w_u^t + W_{imp}^t - W_{proc}^t &\geq 0 & \text{electricity importation and exportation} \\
\sum_{u=1}^{n_u} f_{u, k}^t \cdot w_u^t + W_{imp}^t - W_{prod}^t - W_{proc}^t &\geq 0 & \forall \, t = 1, \ldots, T, \forall \, u \in HU, CU \\
W_{imp}^t &\geq 0 & \forall \, t = 1, \ldots, T, \forall \, u \in HU, CU \\
W_{prod}^t &\geq 0 & \forall \, t = 1, \ldots, T, \forall \, u \in HU, CU \\
F_{min, u} \cdot y_u^t &\leq f_u^t \leq F_{max, u} \cdot y_u^t & \forall \, t = 1, \ldots, T, \forall \, u \in HU, CU \\
f_u - f_u^t &\geq 0 & \forall \, t = 1, \ldots, T, \forall \, u \in FU \\
y_u - y_u^t &\geq 0 & \forall \, t = 1, \ldots, T, \forall \, u \in FU \\
y_u^t &= 0 - 1 & \forall \, u \in FU \\
y_u &= 0 - 1 & \forall \, u \in FU \\
\end{align*}
\]
\[
J_t(x_t) = \left\{ \begin{array}{l}
\sum_{u=1}^{n_u} C_{op, fix, u} \cdot y_u^t + \sum_{t=1}^{t_{\text{times}}} \left( \sum_{u=1}^{n_u} (C_{op, var, u}^t \cdot f_{u, k}^t) + C_{el}^t \cdot W_{imp}^t + p_{el}^t \cdot W_{prod}^t \right) \cdot t_p
\end{array} \right\}
\]
\[
\min_{x_2} \{ J_2(x_2) \}
\]

\[
x_2 = \left\{ \begin{array}{l}
\forall (i, j) \in P_A \\
\forall (i, j) \in P_B \\
\forall i \in H, \forall j \in C : (i, j) \notin P_A, P_B
\end{array} \right. \\
y^0_{ij} \forall i, j \in \mathbb{N} \\
y^1_{ij} \forall i, j \in \mathbb{N} \\
y^2_{ij} \forall i, j \in \mathbb{N}
\right\}
\]

\[
R_{ik} - R_{ik-1} + \sum_{j \in C_k} Q_{i,j,k,z} - \sum_{i \in H_k} Q_{i,j,k,z} = 0 \\
\forall i \in H_k, k \in IT_{zt}, z_t \in IZ_t, t = 1, \ldots, T
\]

Heat balance constraints

\[
\sum_{i \in C_k} Q_{i,j,k,z} = Q_{i,j,k,z} \\
\forall j \in C_k, k \in IT_{zt}, z_t \in IZ_t, t = 1, \ldots, T
\]

Logical Constraints: condition A

\[
\sum_{k \in IZ_t} Q_{i,j,k,z} - U_{ij} y^0_{ij} \leq 0 \\
\forall t = 1, \ldots, T, \forall (i, j) \in P_A
\]

Logical Constraints: condition B

\[
\sum_{k \in IZ_t} Q_{i,j,k,z} - \sum_{z_t \in IZ_t} y_{ij,z_t} \leq 0 \\
\forall t = 1, \ldots, T : t \neq d, \forall z_t \in IZ_t
\]

Logical Constraints generic matches

\[
R_{kzt} \geq 0 \\
Q_{i,j,k,z} \geq 0 \\
\forall z_t \in IZ_t, \forall i \in H_k, \forall j \in C_k, \\
\forall t = 1, \ldots, T, \forall k \in IT_{zt}
\]

Nonnegativity Constraints

\[
y^0_{ij} = 0 - 1 \\
y^1_{ij} = 0 - 1 \\
y^2_{ij} = 0 - 1
\]

0-1 constraints

\[
u_{ij} = y^0_{ij} \quad i \in H, j \in C, (i, j) \in P_A \\
u_{ij} = \sum_{i \in C} y^1_{ij} \quad i \in H, j \in C, (i, j) \in P_B
\]

Constraints for number of units

\[
\sum_{i \in H} \sum_{j \in C} PL_{ij} \cdot u_{ij} \\
\text{with: } PL_{ij} \in [0, 1]
\]

\[J_2(x_2) = \left\{ \begin{array}{l}
\end{array} \right. \]
\[
\begin{align*}
\Omega_3 = & \quad \left\{ f_{b,t}^n \right\} \\
& \quad \left\{ \begin{array}{l}
\sum_{b \in \mathcal{H}^n_{in}(c)} f_{b,t}^n - \sum_{b \in \mathcal{H}^n_{out}(c)} f_{b,t}^n = 0 \\
\forall s \in S_n, \forall n \in \mathcal{HTC}, \forall t = 1, \ldots \text{Times} \\
\sum_{b \in \mathcal{H}^n_{in}(m)} f_{b,t}^n - \sum_{b \in \mathcal{H}^n_{out}(m)} f_{b,t}^n = 0 \\
\forall m \in M_n, \forall n \in \mathcal{HTC}, \forall t = 1, \ldots \text{Times} \\
\sum_{b \in \mathcal{M}^n_{in}(m)} f_{b,t}^n \cdot T_{b,t}^n - \sum_{b \in \mathcal{M}^n_{out}(m)} f_{b,t}^n \cdot T_{b,t}^n = 0 \\
\forall m \in \mathcal{M}_n, \forall n \in \mathcal{HTC}, \forall t = 1, \ldots \text{Times} \\
Q_{ext} - f_{b,t}^n \cdot (T_{in,b}^n - T_{out,b}^n) = 0 \\
\forall ex \in U, \forall i \in \mathcal{H}, \forall t = 1, \ldots \text{Times} \\
Q_{ext} - f_{b,t}^n \cdot (T_{in,b}^n - T_{out,b}^n) = 0 \\
\forall ex \in U, \forall j \in \mathcal{C}, \forall t = 1, \ldots \text{Times} \\
Q_{ext} = \sum_{k \in \mathcal{U}_t} q_{i,k,t} \\
\forall ex \in U, \forall (i,j) \in \mathcal{P}_t \cup \mathcal{I}_t, \forall t = 1, \ldots \text{Times} \\
Q_{ext} = \sum_{ex \in \mathcal{S}_t} q_{i,j,t} \\
\forall ex \in U, \forall (i,j) \in \mathcal{P}_t \cup \mathcal{I}_t, \forall t = 1, \ldots \text{Times} \\
Q_{ext} - U_{\mathcal{A}_{ex}} \cdot LMTD_{ex} \leq 0 \\
\forall ex \in U, \forall t = 1, \ldots \text{Times} \\
(T_{in,b}^n - T_{out,b}^n) \geq \Delta T_{in,b} \\
(T_{in,b}^n - T_{out,b}^n) \geq \Delta T_{in,b} \\
\forall ex \in U, \forall t = 1, \ldots \text{Times} \\
f_{b,t}^n = F_{b,t}^n \\
\forall b \in S_{\mathcal{A}_{ex}}^{in}(m), \forall n \in \mathcal{HTC}, \forall t = 1, \ldots \text{Times} \\
T_{b,t}^n = T_{in}^n \\
\forall b \in S_{\mathcal{A}_{ex}}^{in}(m) \\
T_{b,t}^n = T_{out}^n \\
\forall b \in S_{\mathcal{A}_{ex}}^{out}(m) \\
\forall n \in \mathcal{HTC}, \forall t = 1, \ldots \text{Times} \\
T_{b,t}^n = T_{in}^n \\
\forall b \in S_{\mathcal{A}_{ex}}^{in}(n), \forall i \in S_{\mathcal{A}_{ex}}^{out}(e) \\
\forall n \in \mathcal{HTC}, \forall t = 1, \ldots \text{Times} \\
f_{b,t}^n \geq 0 \\
\forall b \in B^n, \forall n \in \mathcal{HTC}, \forall t = 1, \ldots \text{Times}
\end{array} \right. \\
\end{align*}
\]

\[
J_3(x_3) = \left\{ \sum_{ex \in U} c_{ex} \cdot A_{ex}^B \right\}
\]
Initialization

In this work, dealing with multi-period HENs, a different initialization procedure needs to be used as those for single period problems are not directly applicable. The basic idea is to convert P3 into a simpler problem by:

1) Replacing the objective function of P3 considering the minimization of the sum of the mass flow rates related to the heat exchanger branches \( f_{i,b,t} \).

2) Removing the Heat Exchanger Area constraints (see model P3) and the related variables \( A_{ex}, LMTD_{ex} \).

Observation:

Two Solver Tested:
1) IPOPT (Interior Point based optimization algorithm)
2) SNOPT (SQP optimization algorithm)

IPOPT showed more percentage of converged solutions for the same test cases
3 Bi-level Framework for Multi-period HENS

Mathematical Nature of the Problem:

- Mixed
- Switch on or not?
- Integer
- Size?
- Non
- Load(t) ?
- Linear

Programming

Master Level

Lower Level

*Martelli et Amaldi, 2013*
### Process data:

<table>
<thead>
<tr>
<th>Stream</th>
<th>Q [kW]</th>
<th>Tin [°C]</th>
<th>Tout [°C]</th>
<th>[kW/m2k]</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Period 1</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H1</td>
<td>1522.780</td>
<td>249</td>
<td>100</td>
<td>2</td>
</tr>
<tr>
<td>H2</td>
<td>1658.460</td>
<td>259</td>
<td>128</td>
<td>2</td>
</tr>
<tr>
<td>C1</td>
<td>676.656</td>
<td>96</td>
<td>170</td>
<td>2</td>
</tr>
<tr>
<td>C2</td>
<td>2460</td>
<td>106</td>
<td>270</td>
<td>2</td>
</tr>
<tr>
<td><strong>Period 2</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H1</td>
<td>766.488</td>
<td>229</td>
<td>120</td>
<td>2</td>
</tr>
<tr>
<td>H2</td>
<td>768.040</td>
<td>239</td>
<td>148</td>
<td>2</td>
</tr>
<tr>
<td>C1</td>
<td>676.656</td>
<td>96</td>
<td>170</td>
<td>2</td>
</tr>
<tr>
<td>C2</td>
<td>2460</td>
<td>106</td>
<td>270</td>
<td>2</td>
</tr>
<tr>
<td><strong>Period 3</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H1</td>
<td>1571.950</td>
<td>249</td>
<td>100</td>
<td>2</td>
</tr>
<tr>
<td>H2</td>
<td>1658.460</td>
<td>259</td>
<td>128</td>
<td>2</td>
</tr>
<tr>
<td>C1</td>
<td>207.264</td>
<td>116</td>
<td>150</td>
<td>2</td>
</tr>
<tr>
<td>C2</td>
<td>1240</td>
<td>126</td>
<td>250</td>
<td>2</td>
</tr>
</tbody>
</table>

### Utility data:

<table>
<thead>
<tr>
<th>Utilities</th>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hot Utility (S1)</td>
<td>Tin</td>
<td>300</td>
<td>°C</td>
</tr>
<tr>
<td></td>
<td>Tout</td>
<td>300</td>
<td>°C</td>
</tr>
<tr>
<td></td>
<td>K</td>
<td>1.333</td>
<td>kW/m2k</td>
</tr>
<tr>
<td></td>
<td>C_{op,var,S1}</td>
<td>17.1428</td>
<td>$/MWh</td>
</tr>
<tr>
<td></td>
<td>C_{op,fix,S2}</td>
<td>0</td>
<td>$/MW</td>
</tr>
<tr>
<td>Cold Utility (W1)</td>
<td>Tin [°C]</td>
<td>30</td>
<td>°C</td>
</tr>
<tr>
<td></td>
<td>Tout [°C]</td>
<td>50</td>
<td>°C</td>
</tr>
<tr>
<td></td>
<td>K</td>
<td>0.425</td>
<td>kW/m2k</td>
</tr>
<tr>
<td></td>
<td>C_{op,var,W1}</td>
<td>6.0576</td>
<td>$/MWh</td>
</tr>
<tr>
<td></td>
<td>C_{op,fix,W1}</td>
<td>0</td>
<td>$/MW</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Investment Cost Parameters</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_{ex}$</td>
<td>4333</td>
</tr>
<tr>
<td>$\beta_{ex}$</td>
<td>0.6</td>
</tr>
<tr>
<td>$i$</td>
<td>0.04</td>
</tr>
<tr>
<td>$n$</td>
<td>40</td>
</tr>
</tbody>
</table>

**Additional Constraint:** Forbidden exchange between H1 and C1 process streams (practical reasons, security reasons)

4.1 Results: Best and Sub-optimal solutions

**Best Solution**

<table>
<thead>
<tr>
<th></th>
<th>Objective function: Total Costs [k$]</th>
<th>Operating Costs [k$]</th>
<th>Investment Area Costs [k$]</th>
<th>Discounted Investment Area Costs [k$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>This work</td>
<td>395.14</td>
<td>377.04</td>
<td>362.08</td>
<td>18.10</td>
</tr>
<tr>
<td>Literature Case</td>
<td>482.63</td>
<td>469.16</td>
<td>269.38</td>
<td>13.47</td>
</tr>
</tbody>
</table>

Imprrovement of about **18%** in Objective function

Is the Best Economic Solution also the more practical, secure, controllable?

**Multiple – solutions generation**

<table>
<thead>
<tr>
<th>Sub optimal solutions</th>
<th>Objective function: Total Costs [k$]</th>
<th>Operating Costs [k$]</th>
<th>Investment Area Costs [k$]</th>
<th>Discounted Investment Area Costs [k$]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>395.86</td>
<td>382.45</td>
<td>268.34</td>
<td>13.42</td>
</tr>
<tr>
<td></td>
<td>406.43</td>
<td>395.24</td>
<td>223.89</td>
<td>11.19</td>
</tr>
<tr>
<td></td>
<td>429.24</td>
<td>418.68</td>
<td>211.22</td>
<td>10.56</td>
</tr>
<tr>
<td></td>
<td>446.12</td>
<td>436.63</td>
<td>189.78</td>
<td>9.49</td>
</tr>
<tr>
<td></td>
<td>466.96</td>
<td>457.74</td>
<td>184.46</td>
<td>9.22</td>
</tr>
</tbody>
</table>
4.1 Results: Size, loads at each period, heat exchanger area

**Best Solution: Sizes and heat loads**

<table>
<thead>
<tr>
<th>Match</th>
<th>Period 1</th>
<th>Period 2</th>
<th>Period 3</th>
<th>Heat Exchanger Area [m²]</th>
</tr>
</thead>
<tbody>
<tr>
<td>( S1-C2 )</td>
<td>194.18</td>
<td>1602.128</td>
<td>0</td>
<td>28.76</td>
</tr>
<tr>
<td>( H2-C2-1 )</td>
<td>128.831</td>
<td>0</td>
<td>0</td>
<td>93.48</td>
</tr>
<tr>
<td>( H2-C1 )</td>
<td>676.656</td>
<td>676.656</td>
<td>207.264</td>
<td>21.68</td>
</tr>
<tr>
<td>( H2-C2-2 )</td>
<td>852.973</td>
<td>91.384</td>
<td>1240</td>
<td>104.93</td>
</tr>
<tr>
<td>( H1-C2 )</td>
<td>1287.02</td>
<td>766.488</td>
<td>0</td>
<td>246.46</td>
</tr>
<tr>
<td>( H2-W1 )</td>
<td>0</td>
<td>0</td>
<td>211.196</td>
<td>4.11</td>
</tr>
<tr>
<td>( H1-W1 )</td>
<td>238.764</td>
<td>0</td>
<td>1571.95</td>
<td>36.43</td>
</tr>
</tbody>
</table>

* line denotes division between zones

Hot utility size: 1600 kW

Cold Utility size: 1780 kW

Forbidden Exchange is respected
4.1 Results: Network superstructure in Period 1
4.1 Results: Network superstructure in Period 2
4.1 Results: Network Superstructure in Period 3
The proposed framework allows to:

- Select and size Plant Utilities;
- Schedule utility systems with respect of OPEX;
- Design the Heat Exchanger Network, by minimizing Total Yearly Costs (OPEX – CAPEX);
- Practical/engineering constraints are included, such as:
  - Forbidden Exchanges
  - Restricted Exchanges
  - Minimum/Maximum loads between matches

Work in Progress:
- Extend this framework including thermal storages as utilities;
- Extend this framework for Multi Objective stochastic optimization;
Thanks for your attention!

Questions?

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