Parameter Estimation of Complicated Thermodynamic Models for Accurate Brine Separation

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Session : Industrial Applied Mathematics

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2023 AIChE ANNUAL MEETING

UCONN UNIVERSITY OF CONNECTICUT

Process Systems and Operations Research Laboratory

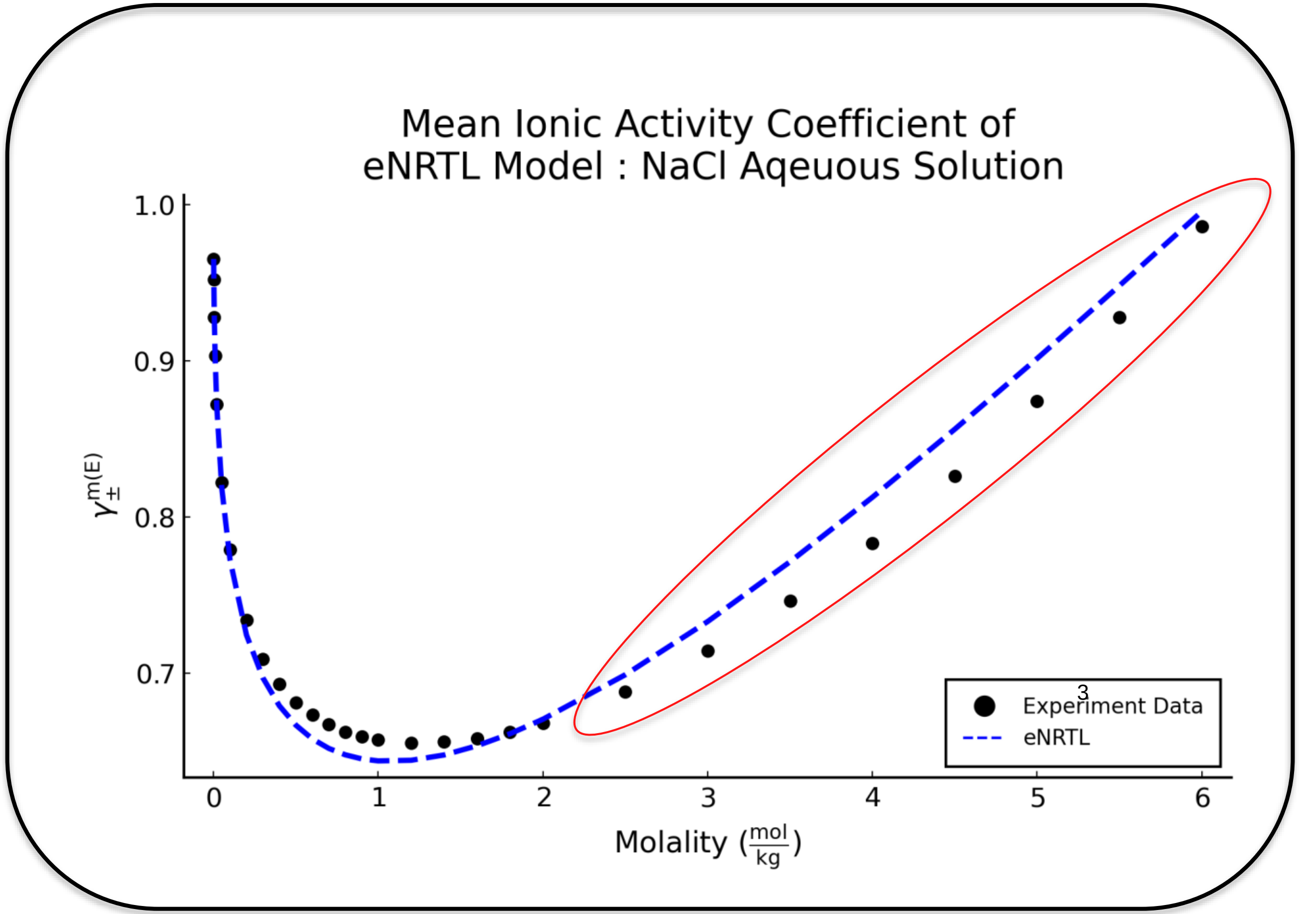
Motivation

Brine separation is of critical importance to many industries with **brine effluent streams** and/or **brine concentration needs** (e.g., agriculture, power production, mining)

- Reduce costs
- Improve system robustness
- Increase sustainability

[1] Molinari, Raffaele., et al. **"Can brine from seawater desalination plants Be a source of critical metals?."** *CHEMVIEWS* (2022).
[2] Stuber, Matthew D., et al. **"Pilot demonstration of concentrated solar-powered desalination of subsurface agricultural drainage water and other brackish groundwater sources."** *Desalination* 355 (2015): 186-196.

Motivation



[3] Song, Yuhua, et al. **"Symmetric electrolyte nonrandom two-liquid activity coefficient model."** *Industrial & Engineering Chemistry Research* 48, no. 16 (2009): 7788-7797.

Refined eNRTL

4

Short Range Interaction

Long Range Interaction

Born term, for aqueous system = 0

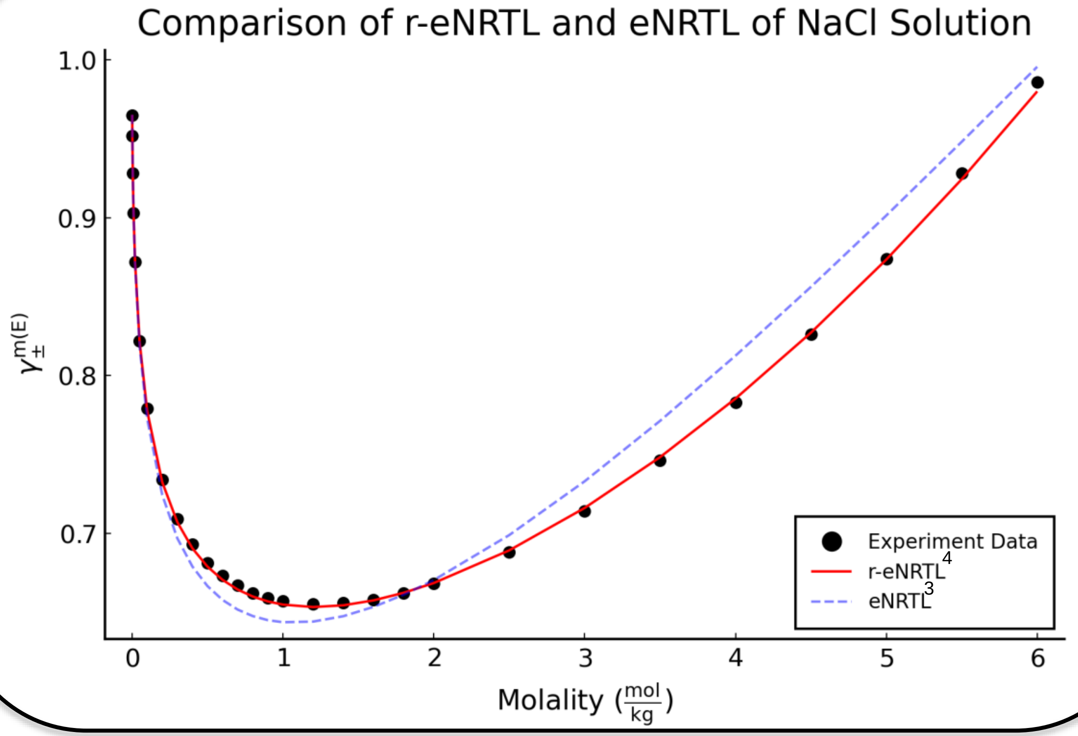
$$G^{*,ex} = G^{*,SR} + G^{*,LR} + \Delta G^{*,Born}$$

$$= G^{*,SR} + (A^{*,LR} + PV) + 0$$

- Increase accuracy of thermodynamic properties calculation
- Improve accuracy of simulation results

[4] Bollas, G.M., et al. **Refined electrolyte-NRTL model: Activity coefficient expressions for application to multi-electrolyte systems**. *AIChE Journal* 54(6): 1608-1624 (2008).

Motivation



Modeling accuracy in high concentration regime

- Refined e-NRTL[3]

[4] Bollas, G.M., et al. **Refined electrolyte-NRTL model: Activity coefficient expressions for application to multi-electrolyte systems**. *AIChE Journal* 54(6): 1608-1624 (2008).

Complexity of Refined eNRTL

$$
\begin{aligned}
\frac{G^{\mathrm{SR}}}{RT} = {} & \sum_{j=1}^{n_m} X_{m_j} \left(\frac{\sum_{s\in\{m,a,c\}} \sum_{l=1}^{n_s} X_{s_l} F_{m_j,s_l,m_j} \tau_{m_j,s_l,m_j}}{\sum_{s\in\{m,a,c\}} \sum_{l=1}^{n_s} X_{s_l} F_{m_j,s_l,m_j}} \right) \\
& + \sum_{j=1}^{n_a} X_{a_j} \sum_{k=1}^{n_c} \left(\frac{X_{c_k}}{\sum_{k'=1}^{n_c} X_{c_{k'}}} \right) \left(\frac{\sum_{s\in\{m,c\}} \sum_{l=1}^{n_s} X_{s_l} F_{a_j,s_l,c_k} \tau_{a_j,s_l,c_k}}{\sum_{s\in\{m,c\}} \sum_{l=1}^{n_s} X_{s_l} F_{a_j,s_l,c_k}} \right) \\
& + \sum_{j=1}^{n_c} X_{c_j} \sum_{k=1}^{n_a} \left(\frac{X_{a_k}}{\sum_{k'=1}^{n_a} X_{a_{k'}}} \right) \left(\frac{\sum_{s\in\{m,a\}} \sum_{l=1}^{n_s} X_{s_l} F_{c_j,s_l,a_k} \tau_{c_j,s_l,a_k}}{\sum_{s\in\{m,a\}} \sum_{l=1}^{n_s} X_{s_l} F_{c_j,s_l,a_k}} \right)
\end{aligned}
$$

$$
\log \gamma_{t_j}^{\mathrm{SR}} = \frac{\partial}{\partial N_{t_j}} \left(\sum_{\hat{t}\in\{m,a,c\}} \sum_{\hat{j}=1}^{n_{\hat{t}}} N_{\hat{t}_{\hat{j}}} \frac{G^{\mathrm{SR}}}{RT} \right)
$$

[5] Gottlieb, Robert X., et al. "**Automatic Source Code Generation of Complicated Models For Deterministic Global Optimization With Parallel Architectures**."

Complexity of Refined eNRTL

$$\frac{G^{\mathrm{SR}}}{RT} = \sum_{j=1}^{n_m} X_{m_j} \left(\frac{\sum_{s\in\{m,a,c\}} \sum_{l=1}^{n_s} X_{s_l} F_{m_j,s_l,m_j} \tau_{m_j,s_l,m_j}}{\sum_{s\in\{m,a,c\}} \sum_{l=1}^{n_s} X_{s_l} F_{m_j,s_l,m_j}} \right)$$
$$+ \sum_{j=1}^{n_a} X_{a_j} \sum_{k=1}^{n_c} \left(\frac{X_{c_k}}{\sum_{k'=1}^{n_c} X_{c_{k'}}} \right) \left(\frac{\sum_{s\in\{m,c\}} \sum_{l=1}^{n_s} X_{s_l} F_{a_j,s_l,c_k} \tau_{a_j,s_l,c_k}}{\sum_{s\in\{m,c\}} \sum_{l=1}^{n_s} X_{s_l} F_{a_j,s_l,c_k}} \right)$$
$$+ \sum_{j=1}^{n_c} X_{c_j} \sum_{k=1}^{n_a} \left(\frac{X_{a_k}}{\sum_{k'=1}^{n_a} X_{a_{k'}}} \right) \left(\frac{\sum_{s\in\{m,a\}} \sum_{l=1}^{n_s} X_{s_l} F_{c_j,s_l,a_k} \tau_{c_j,s_l,a_k}}{\sum_{s\in\{m,a\}} \sum_{l=1}^{n_s} X_{s_l} F_{c_j,s_l,a_k}} \right)$$

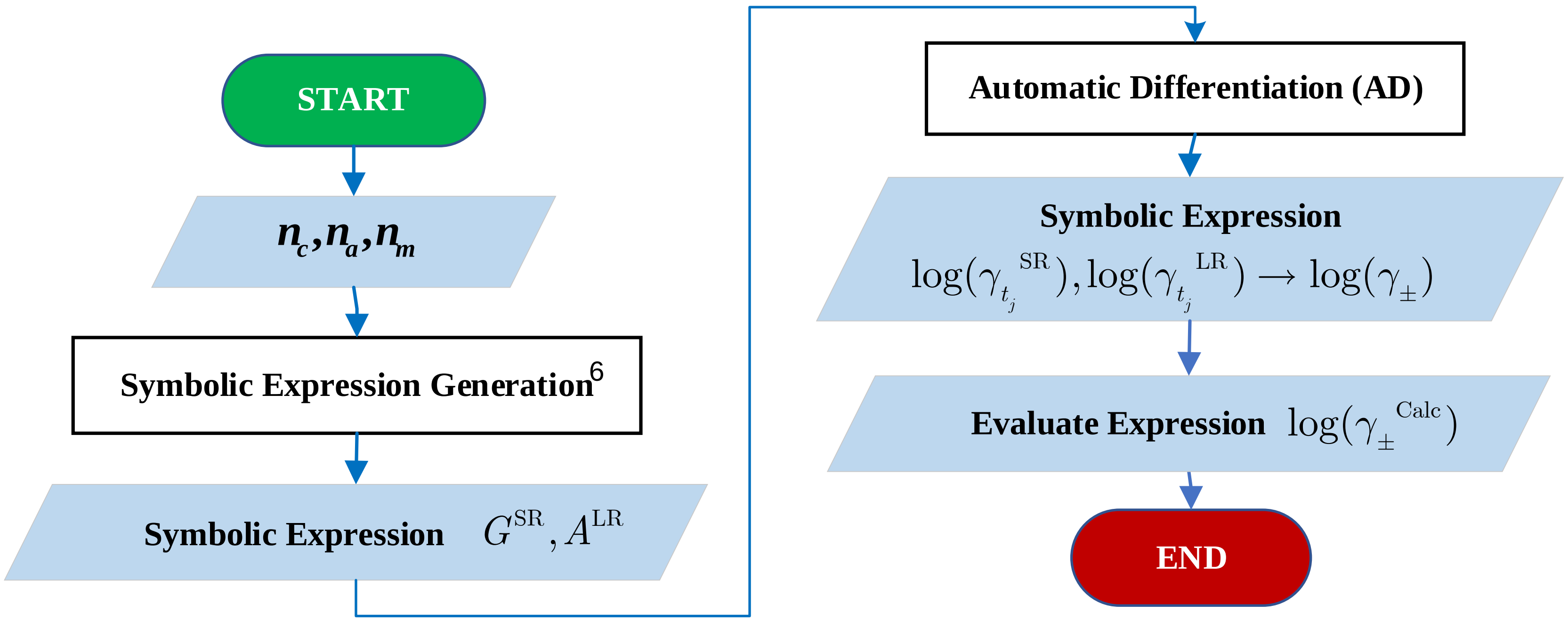
$$\log \gamma_{t_j}^{\mathrm{SR}} = \frac{\partial}{\partial N_{t_j}} \left(\sum_{\hat{t}\in\{m,a,c\}} \sum_{\hat{j}=1}^{n_{\hat{t}}} N_{\hat{t}_{\hat{j}}} \frac{G^{\mathrm{SR}}}{RT} \right)$$

AD

Complicated Expression

[5] Gottlieb, Robert X., et al. "**Automatic Source Code Generation of Complicated Models For Deterministic Global Optimization With Parallel Architectures**."

Automatic Differentiation Workflow



n_c, n_a, n_m: Number of species in aqueous phase.

G^{SR}: Short range excess Gibbs free energy.

A^{LR}: Long range excess Helmholtz free energy.

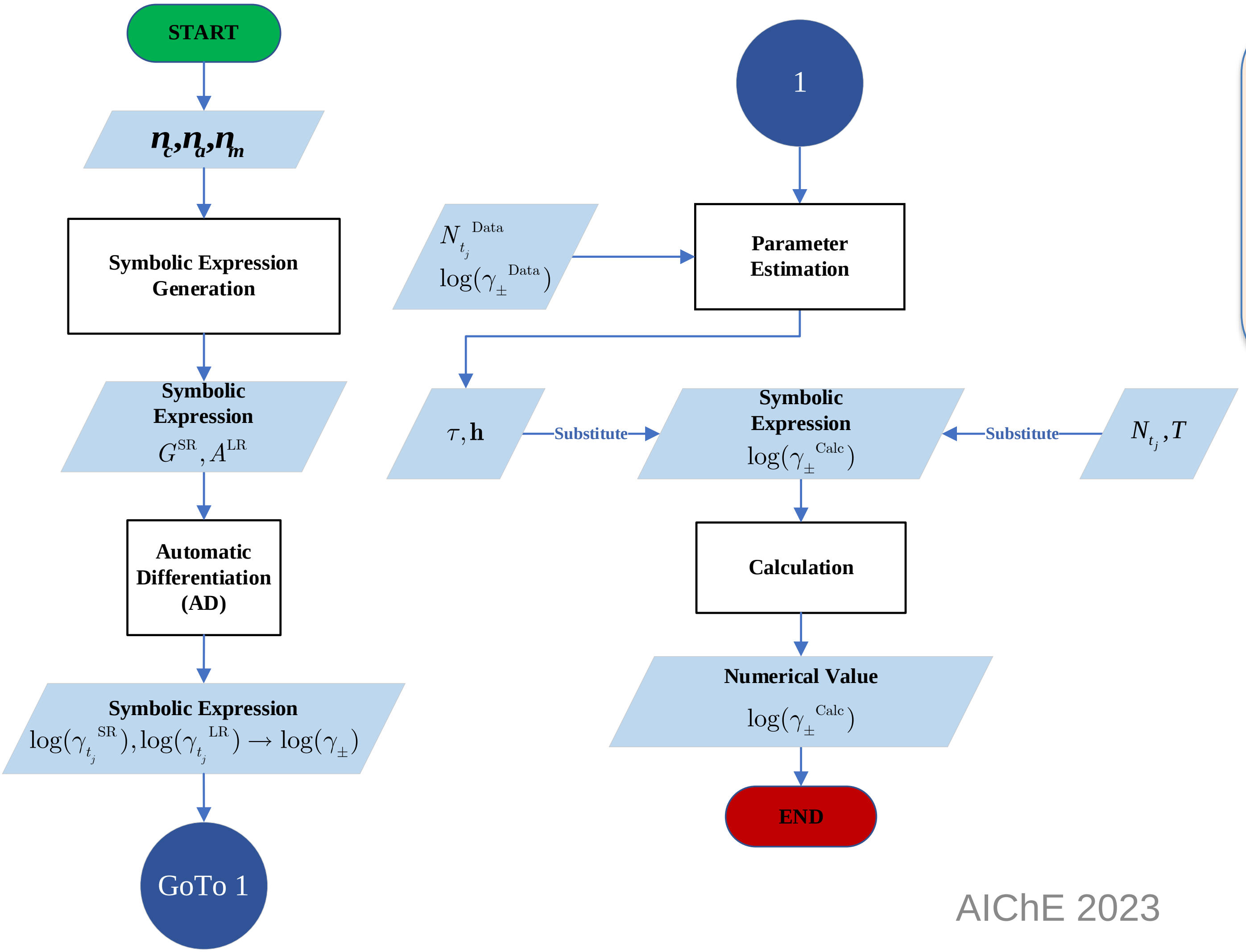
$\gamma_{t_j}^{SR}$: Short Range activity coefficient of species t_j.

$\gamma_{t_j}^{LR}$: Long Range activity coefficient of species t_j.

t_j: Species with type t, $t \in \{a, c, m\}$ and index j.

[6] Gowda, S., et al. **"High-performance symbolic-numerics via multiple dispatch."** *ACM Communications in Computer Algebra* 55, no. 3 (2022): 92-96.

R-eNRTL Parameter Estimation



$$
\begin{aligned}
\mathbf{p}^* \in \arg \min_{\mathbf{p} \in P \subset \mathbb{R}^{n_p}} & \sum_{i=1}^{n_d} \left(y_i(\mathbf{p}) - y_i^{\text{data}}\right)^2 \\
\text{s.t.} \quad & \mathbf{h}(\mathbf{p}) = \mathbf{0} \\
& \mathbf{g}(\mathbf{p}) \leq \mathbf{0}
\end{aligned}
$$

- **n_c, n_a, n_m:** Number of species in aqueous phase.
- **G^{SR}:** Short range excess Gibbs free energy.
- **A^{LR}:** Long range excess Helmholtz free energy.
- **$\gamma_{t_j}^{SR}$:** Short Range activity coefficient of species t_j.
- **$\gamma_{t_j}^{LR}$:** Long Range activity coefficient of species t_j.
- **t_j:** Species with type t, $t \in \{a, c, m\}$ and index j.
- **$N_{t_j}^{Data}$:** Experimental data of concentrations of each species.
- **$\gamma_{\pm}^{Data}$:** Experimental data of mean molal activity coefficient
- **h:** Hydration number of each species, design variables for parameter estimation
- **τ:** Interaction parameters, design variables for parameter estimation
- **N_{t_j}:** The concentration of each species in object system

R-eNRTL Parameter Estimation

$$
\begin{aligned}
\frac{G^{\mathrm{SR}}}{RT} = \sum_{j=1}^{n_m} X_{m_j} \left(\frac{\sum_{s\in\{m,a,c\}} \sum_{l=1}^{n_s} X_{s_l} F_{m_j,s_l,m_j} \tau_{m_j,s_l,m_j}}{\sum_{s\in\{m,a,c\}} \sum_{l=1}^{n_s} X_{s_l} F_{m_j,s_l,m_j}} \right) \\
+ \sum_{j=1}^{n_a} X_{a_j} \sum_{k=1}^{n_c} \left(\frac{X_{c_k}}{\sum_{k'=1}^{n_c} X_{c_{k'}}} \right) \left(\frac{\sum_{s\in\{m,c\}} \sum_{l=1}^{n_s} X_{s_l} F_{a_j,s_l,c_k} \tau_{a_j,s_l,c_k}}{\sum_{s\in\{m,c\}} \sum_{l=1}^{n_s} X_{s_l} F_{a_j,s_l,c_k}} \right) \\
+ \sum_{j=1}^{n_c} X_{c_j} \sum_{k=1}^{n_a} \left(\frac{X_{a_k}}{\sum_{k'=1}^{n_a} X_{a_{k'}}} \right) \left(\frac{\sum_{s\in\{m,a\}} \sum_{l=1}^{n_s} X_{s_l} F_{c_j,s_l,a_k} \tau_{c_j,s_l,a_k}}{\sum_{s\in\{m,a\}} \sum_{l=1}^{n_s} X_{s_l} F_{c_j,s_l,a_k}} \right)
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{p}^* \in \arg \min_{\mathbf{p}\in P\subset\mathbb{R}^{n_p}} \sum_{i=1}^{n_d} \left(y_i(\mathbf{p}) - y_i^{\mathrm{data}}\right)^2 \\
\text{s.t.} \quad \mathbf{h}(\mathbf{p}) = \mathbf{0} \\
\mathbf{g}(\mathbf{p}) \leq \mathbf{0}
\end{aligned}
$$

N_{t_j}, T

n_c, n_a, n_m: Number of species in aqueous phase.

$$
F_{a_j,s_l,c_k} = \exp(-0.2\tau_{a_j,s_l,c_k})
$$

timation

τ: Interaction parameters, design variables for parameter estimation

N_{t_j}: The concentration of each species in object system

EAGO.jl

Deterministic global optimizer

- High performance
- Open-source and free for non-commercial use
- Extensible
- Interval Arithmetic & McCormick based relaxation library

https://www.github.com/PSORLab/EAGO.jl

[7] Wilhelm, Matthew E., and Matthew D. Stuber. **"EAGO. jl: easy advanced global optimization in Julia."** *Optimization Methods and Software* 37, no. 2 (2022): 425-450.

Challenge: Dependency Problem

$$f(x) = \frac{\exp(x)}{\exp(x)} = 1$$

$$F(X) = \frac{\exp(X)}{\exp(X)} = \left[\frac{\exp(x^L)}{\exp(x^U)}, \frac{\exp(x^U)}{\exp(x^L)}\right]$$

$$X = [-5, 5]$$

$$\Rightarrow$$

$$\left[\frac{\exp(-5)}{\exp(5)}, \frac{\exp(5)}{\exp(-5)}\right]$$

Challenge: Dependency Problem

$$f(x) = \frac{\exp(x)}{\exp(x)} = 1$$

$$F(X) = \frac{\exp(X)}{\exp(X)} = \left[\frac{\exp(x^L)}{\exp(x^U)}, \frac{\exp(x^U)}{\exp(x^L)}\right]$$

$$X = [-5, 5]$$

$$\Rightarrow \left[4.5 \times 10^{-5}, 2.2 \times 10^{4}\right]$$

Challenge: Dependency Problem

Abstracted Form of Problematic Terms

$$\left(\frac{\sum_{j=1}^{n} \exp(x_j)x_j}{\sum_{j=1}^{n} \exp(x_j)}\right)$$

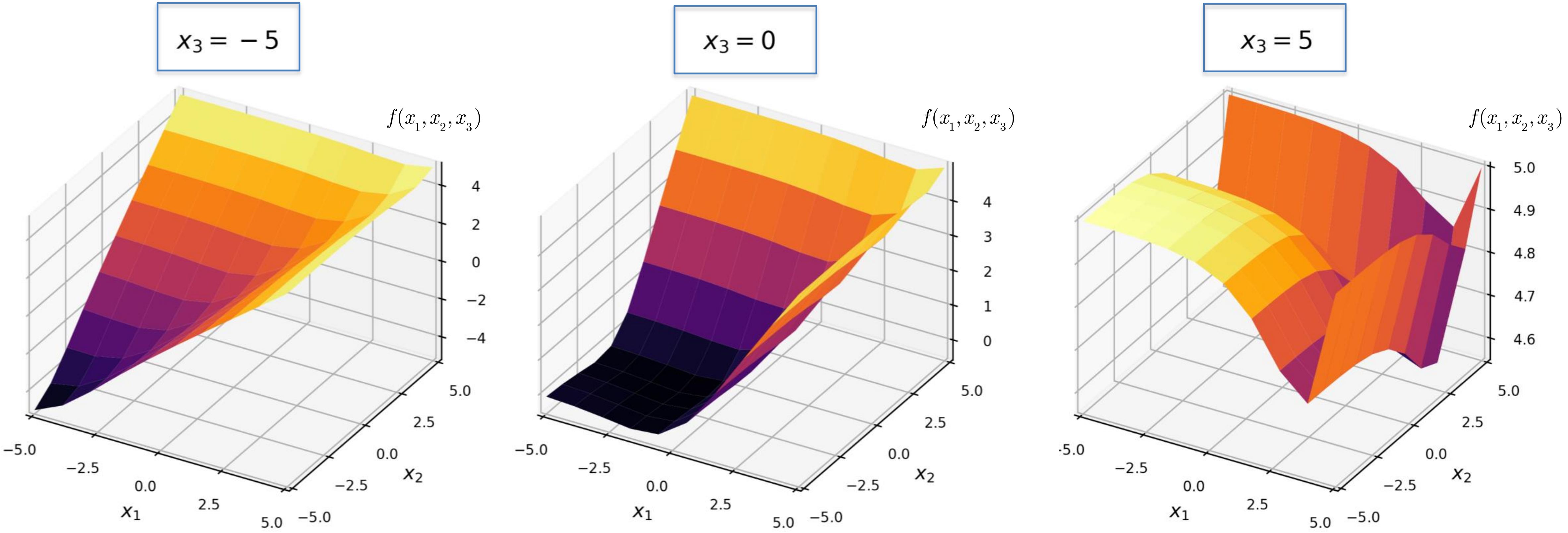
EX: Single Term

$$X = [x^L, x^U]$$

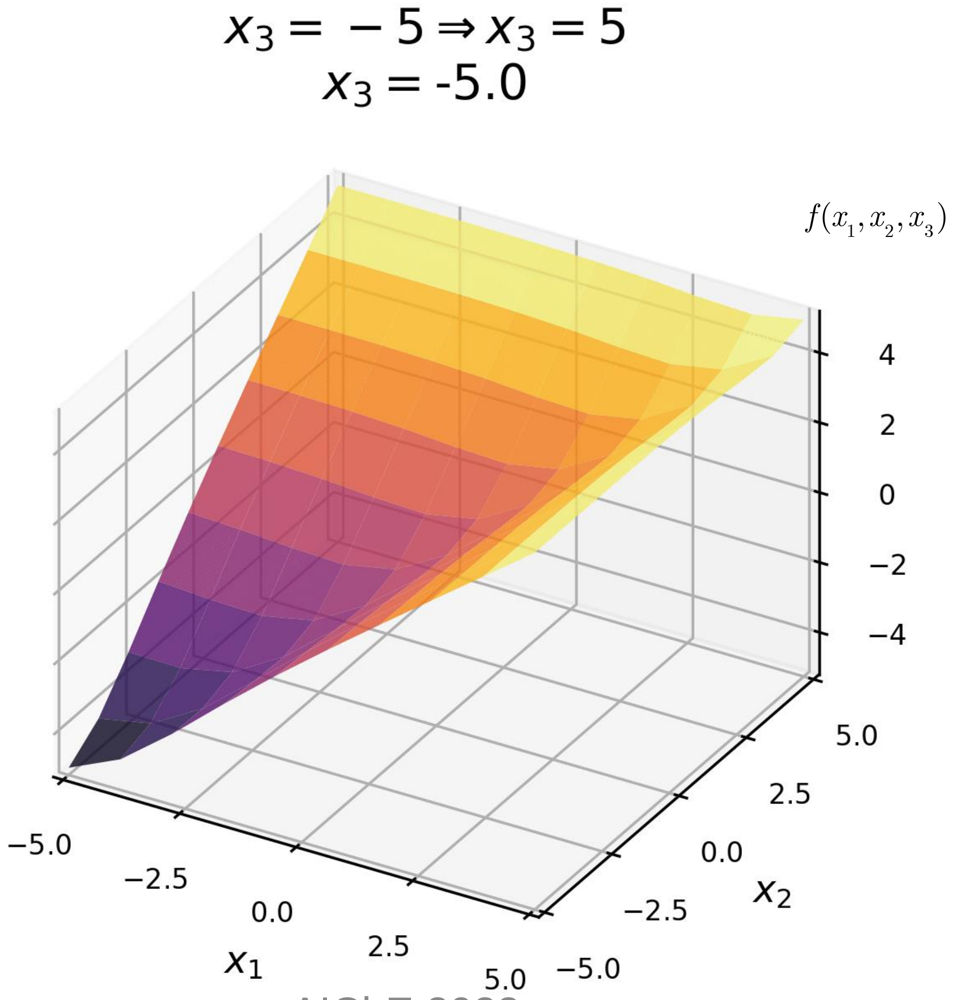
$$\frac{\exp(X)}{\exp(X)} = \left[\frac{\exp(x^L)}{\exp(x^U)}, \frac{\exp(x^U)}{\exp(x^L)}\right]$$

$$\frac{X\exp(X)}{\exp(X)} = \left[\min\left\{\frac{x^L\exp(x^U)}{\exp(x^L)}, \frac{x^L\exp(x^L)}{\exp(x^L)}\right\}, \max\left\{\frac{x^U\exp(x^U)}{\exp(x^L)}, \frac{x^U\exp(x^L)}{\exp(x^L)}\right\}\right]$$

Function Profile (n=3)



Function Profile Animation



Interval Extension (n=3)

$$f(\mathbf{x}) = \frac{\mathbf{x}^{\mathrm{T}} \exp(\mathbf{x})}{\mathbf{1}^{\mathrm{T}} \exp(\mathbf{x})}$$

Domain

$$X_1, X_2, X_3 = [-5, 5]$$

Interval Arithmetic

$$F \;\; X = \left[3\frac{-5\exp(5)}{\exp(-5)}, 3\frac{5\exp(5)}{\exp(-5)}\right]$$

$$\approx [-3\times 10^5, 3\times 10^5]$$

5 orders of magnitude larger than the interval hull of the image set

$$\hat{f}(X) = [-5, 5]$$

A Tight Interval Extension Rule

$$f(\mathbf{x}) = \frac{\mathbf{x}^{\mathbf{T}} \exp(\mathbf{x})}{\mathbf{1}^{\mathrm{T}} \exp(\mathbf{x})} = \frac{x_1 \exp(x_1) + x_2 \exp(x_2) + \ldots + x_n \exp(x_n)}{\exp(x_1) + \exp(x_2) + \ldots + \exp(x_n)} = \sum_{i=1}^{n} \frac{x_i \exp(x_i)}{\sum_{j=1}^{n} \exp(x_j)}$$

A Tight Interval Extension Rule

$$f(\mathbf{x}) = \frac{\mathbf{x}^{\mathrm{T}} \exp(\mathbf{x})}{\mathbf{1}^{\mathrm{T}} \exp(\mathbf{x})} = \frac{x_1 \exp(x_1) + x_2 \exp(x_2) + \ldots + x_n \exp(x_n)}{\exp(x_1) + \exp(x_2) + \ldots + \exp(x_n)} = \sum_{i=1}^{n} \frac{x_i \exp(x_i)}{\sum_{j=1}^{n} \exp(x_j)}$$

$$\sum_{i=1}^{n} \frac{x_i \exp(x_i)}{\exp(x_1) + \exp(x_2) + \ldots + \exp(x_n)} \cdot \frac{\exp(-x_i)}{\exp(-x_i)} = \sum_{i=1}^{n} \frac{x_i}{\exp(x_1 - x_i) + \exp(x_2 - x_i) + \ldots + \exp(x_n - x_i)}$$

A Tight Interval Extension Rule

$$f(\mathbf{x}) = \frac{\mathbf{x}^{\mathrm{T}} \exp(\mathbf{x})}{\mathbf{1}^{\mathrm{T}} \exp(\mathbf{x})} = \frac{x_1 \exp(x_1) + x_2 \exp(x_2) + \ldots + x_n \exp(x_n)}{\exp(x_1) + \exp(x_2) + \ldots + \exp(x_n)} = \sum_{i=1}^{n} \frac{x_i \exp(x_i)}{\sum_{j=1}^{n} \exp(x_j)}$$

$$\sum_{i=1}^{n} \frac{x_i \exp(x_i)}{\exp(x_1) + \exp(x_2) + \ldots + \exp(x_n)} \cdot \frac{\exp(-x_i)}{\exp(-x_i)} = \sum_{i=1}^{n} \frac{x_i}{\exp(x_1 - x_i) + \exp(x_2 - x_i) + \ldots + \exp(x_n - x_i)}$$

$$\sum_{i=1}^{n} \frac{x_i}{\exp(x_1 - x_i) + \exp(x_2 - x_i) + \ldots + \exp(x_n - x_i)}$$

$$\Rightarrow f(\mathbf{x}) = \sum_{i=1}^{n} \frac{x_i}{1 + \sum_{\substack{j=1 \\ j \neq i}}^{n} \exp(x_j - x_i)}$$

A Tight Interval Extension Rule

$$f(\mathbf{x}) = \frac{\mathbf{x}^{\mathrm{T}} \exp(\mathbf{x})}{\mathbf{1}^{\mathrm{T}} \exp(\mathbf{x})} = \frac{x_1 \exp(x_1) + x_2 \exp(x_2) + \ldots + x_n \exp(x_n)}{\exp(x_1) + \exp(x_2) + \ldots + \exp(x_n)} = \sum_{i=1}^{n} \frac{x_i \exp(x_i)}{\sum_{j=1}^{n} \exp(x_j)}$$

$$\sum_{i=1}^{n} \frac{x_i \exp(x_i)}{\exp(x_1) + \exp(x_2) + \ldots + \exp(x_n)} \cdot \frac{\exp(-x_i)}{\exp(-x_i)} = \sum_{i=1}^{n} \frac{x_i}{\exp(x_1 - x_i) + \exp(x_2 - x_i) + \ldots + \exp(x_n - x_i)}$$

$$\sum_{i=1}^{n} \frac{x_i}{\exp(x_1 - x_i) + \exp(x_2 - x_i) + \ldots + \exp(x_n - x_i)}$$

$$\Rightarrow f(\mathbf{x}) = \sum_{i=1}^{n} \frac{x_i}{1 + \sum_{\substack{j=1 \\ j \neq i}}^{n} \exp(x_j - x_i)}$$

- After conversion, although terms become more complex, the exponential terms in the numerator have been eliminated.
- Only denominator contains exponential terms.

A Tight Interval Extension Rule

$$X_1, X_2, X_3 = [-5, 5]$$

$$f(\mathbf{x}) = \frac{\mathbf{x}^{\mathrm{T}} \exp(\mathbf{x})}{\mathbf{1}^{\mathrm{T}} \exp(\mathbf{x})}$$

$$\Rightarrow$$

$$F \;\; X = \left[3\frac{-5\exp(5)}{\exp(-5)}, 3\frac{5\exp(5)}{\exp(-5)}\right] \approx \left[-3\times 10^5, 3\times 10^5\right]$$

$$f(\mathbf{x}) = \sum_{i=1}^{3} \frac{x_i}{1 + \sum_{j=1, j\neq i}^{n} \exp(x_j - x_i)}$$

$$\Rightarrow$$

$$F \;\; X = \left[3\frac{-5}{1+2\exp(-5-5)}, 3\frac{5}{1+2\exp(-5-5)}\right] \approx [\text{-}15, 15]$$

A Tight Interval Extension Rule

$$X_1, X_2, X_3 = [-5, 5]$$

$$f(\mathbf{x}) = \frac{\mathbf{x}^{\mathrm{T}} \exp(\mathbf{x})}{\mathbf{1}^{\mathrm{T}} \exp(\mathbf{x})}$$

$\Rightarrow$

$$F(X) = \left[3\frac{-5\exp(5)}{\cdots}, 3\frac{5\exp(5)}{\cdots}\right]$$

$$f(\mathbf{x}) = \sum_{i=1}^{3} \frac{x_i}{1 + \sum_{j=1, j\neq i}^{n} \exp(x_j - x_i)}$$

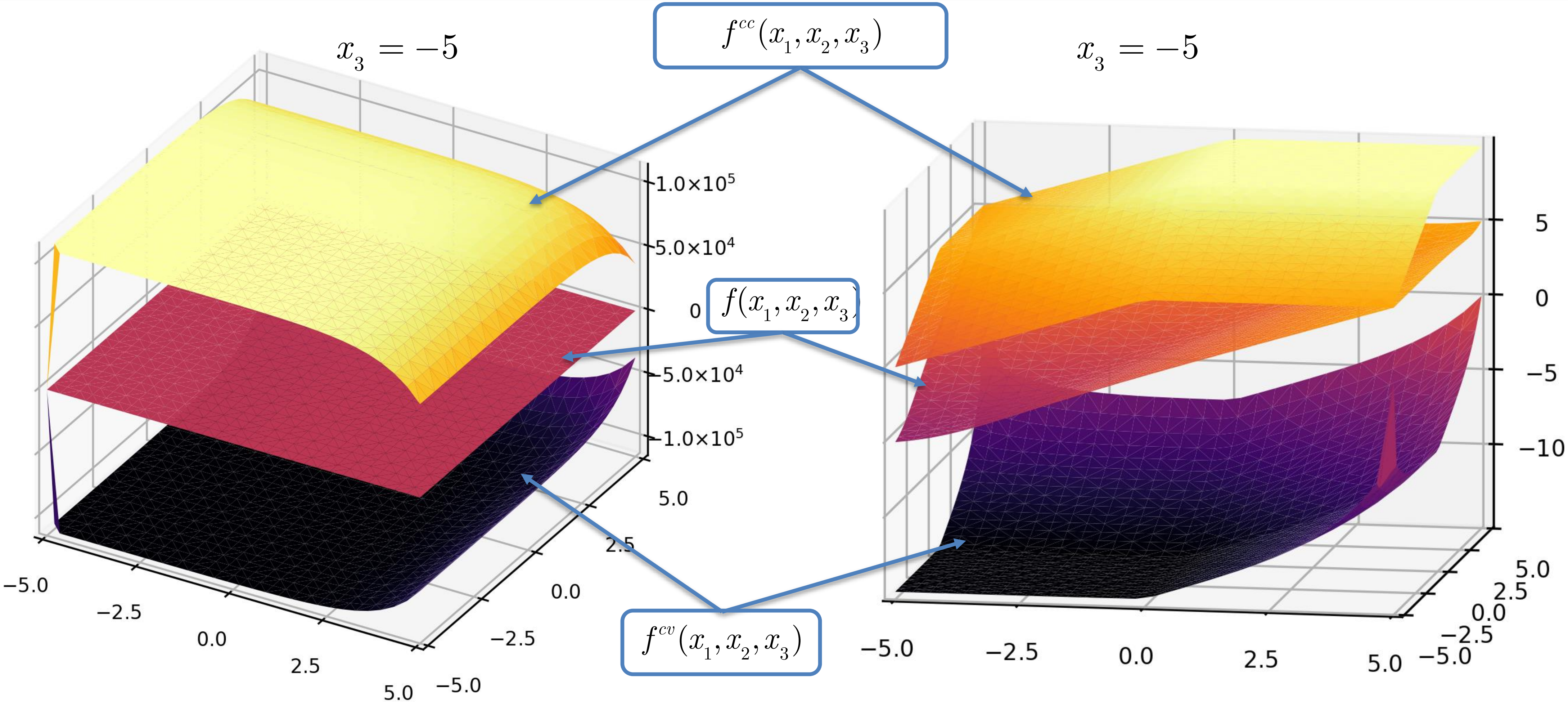
$\Rightarrow$

$$F(X) = \left[\cdots -5-5)}\right]$$

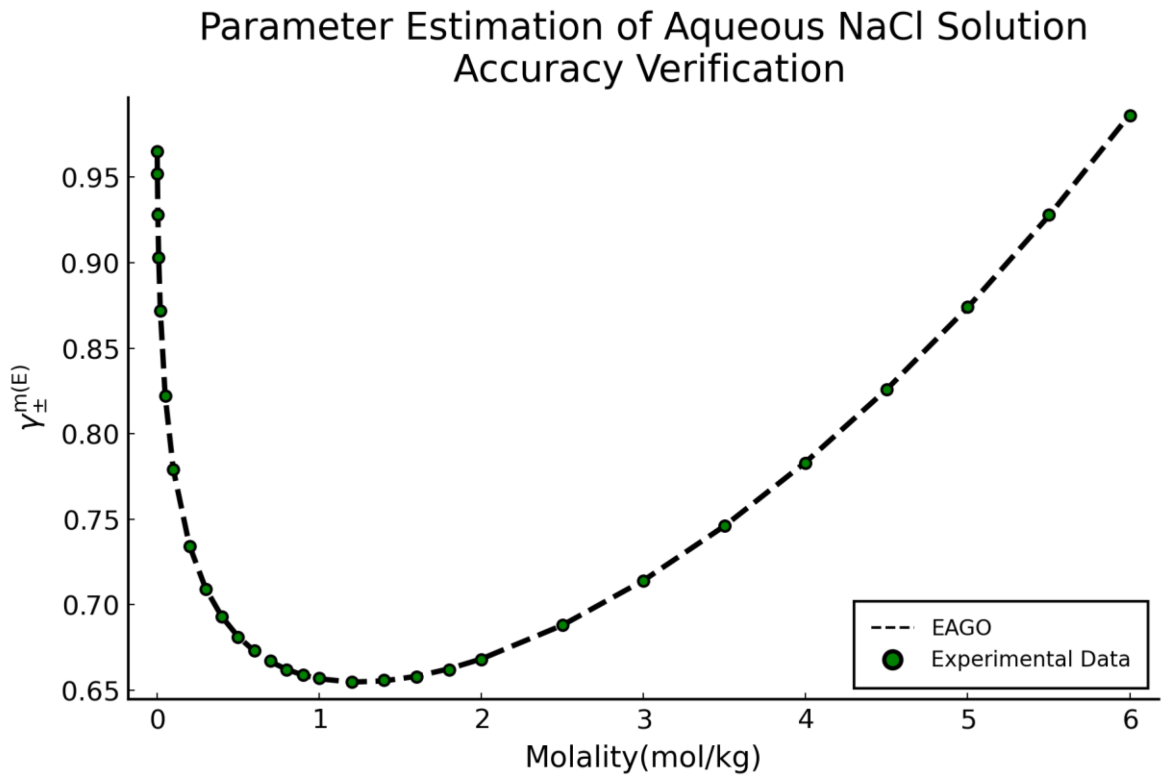
$$\approx [\cdots]$$

Interval shrunk by **4** orders of magnitude

McCormick Relaxations



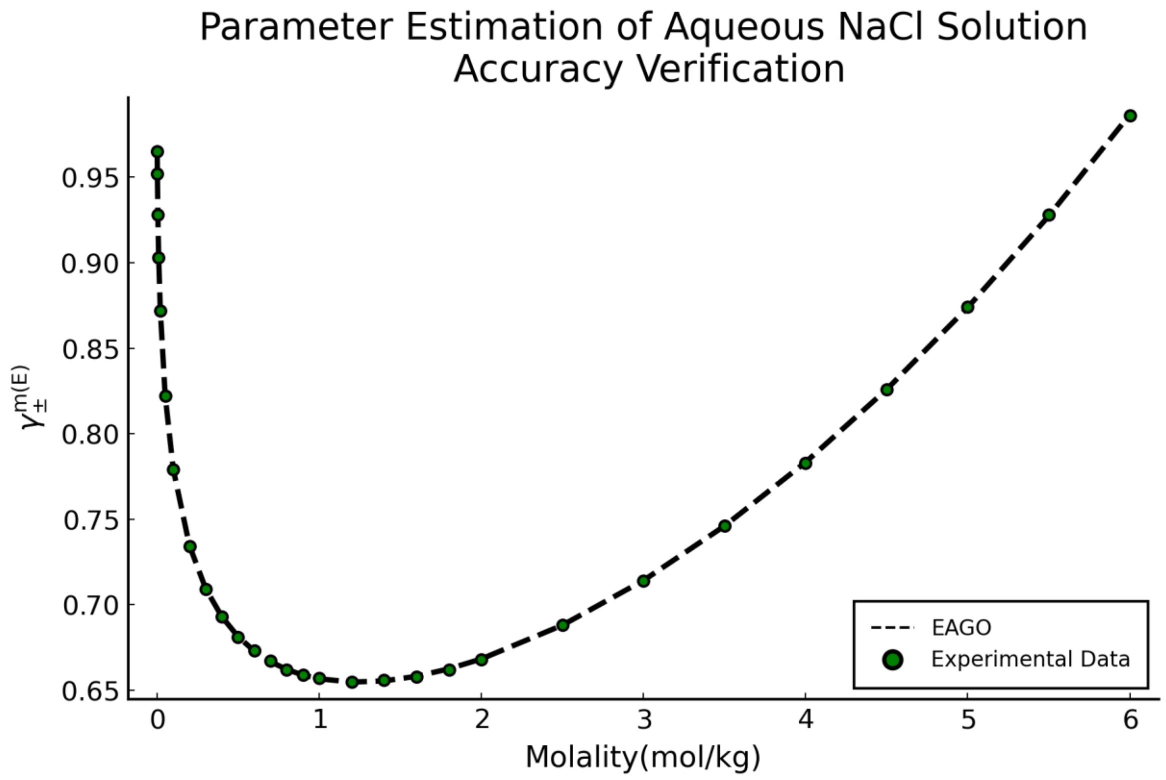
Parameter Estimation Result




```
using JuMP, EAGO, ForwardDiff
import JuMP.@variable as @variable
new_fun = functionalize_obj_NaCl_fast(expr)
objfun(τ1,τ2,hc11,ha11) = objfun_eval_single_γˢᴿ_NaCl_fast(new_fun,τ1,τ2,hc11,ha11)
factory = () -> EAGO.Optimizer(SubSolvers())
model = Model(optimizer_with_attributes(factory, "absolute_tolerance" => 1e-4,"time_
register(model,:objfun,4,objfun,autodiff=true)
lb =[0. -10. 0. 0.]
ub = [10. 0. 2. 2.]
@variable(model, lb[i]<= x[i=1:4] <= ub[i] )
@NLobjective(model, Min, objfun(x[1], x[2], x[3], x[4]))
@NLconstraint(model, y1, x[3]-x[4]>=0)
optimize!(model)
```

✓ 9m 45.1s

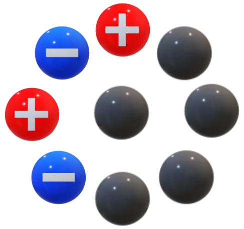
Parameter Estimation Result




```
Absolute Tolerance Achieved
First Solution Found at Node 1029
LBD = 0.0
UBD = 5.977314675518958e-6
Solution is:
    X[1] = 7.834167504201094
    X[2] = -3.907172657309239
    X[3] = 1.5789380575987575
    X[4] = 0.723255866122256
```

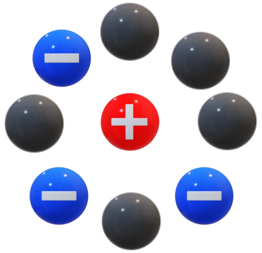
Scalability

Interaction Parameter



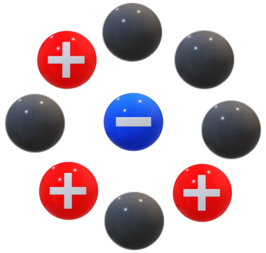
Neutral Species Centered (3 Types of Species Around)

$$2n_m n_a n_c$$



Cation Centered (2 Types of Species Around)

$$\frac{1}{2} n_c n_a (n_a - 1)$$



Anion Centered (2 Types of Species Around)

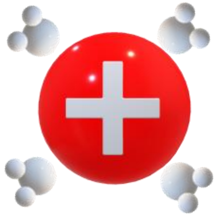
$$\frac{1}{2} n_a n_c (n_c - 1)$$

Total number of parameters

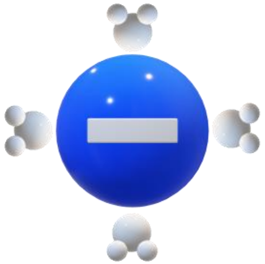
$$\frac{1}{2} n_c n_a (n_c - 1) + \frac{1}{2} n_a n_c (n_a - 1) + 2 n_c n_a n_m + n_c + n_a$$

For a system with 10 unique species each of anions and cations, water as solvent, there are **1120** parameters to fit

Hydration number $\mathbf{h}_c, \mathbf{h}_a$



n_c



n_a

Conclusions

- Implemented refined eNRTL model for single electrolyte case and generated activity coefficients as symbolic expressions using AD.

- Reformulated problematic multivariate quotient term to significantly reduce overestimation of dependency problems.

- Demonstrated the new rule by solving the parameter estimation problem for aqueous NaCl using EAGO.

- Currently implementing the multi-electrolyte form and expanding the AD work for all other thermodynamic properties

Thanks!

2023 AIChE ANNUAL MEETING

Members of the Process Systems and Operations Research Laboratory at the University of Connecticut (https://psor.uconn.edu/)

NAWI National Alliance for Water Innovation

Process Systems and Operations Research Laboratory

Funding:

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Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Alliance for Water Innovation or the U.S. government.

Questions

Process Systems and
Operations Research
Laboratory

https://www.psor.uconn.edu

Thermodynamic of Refined eNRTL

Short Range Interaction

Long Range Interaction

Born term, for aqueous system = 0

$$G^{*,ex} = G^{*,SR} + G^{*,LR} + \Delta G^{*,Born}$$

$$= G^{*,SR} + (A^{*,LR} + PV) + 0$$

$$\ln \gamma_j^*(T,P,x) \equiv \frac{1}{RT}\left(\frac{\partial G^{*,ex}}{\partial N_j}\right)_{T,P,N_{k\neq j}}$$

$$= \frac{1}{RT}\left(\left(\frac{\partial G^{*,SR}}{\partial N_j}\right)_{T,P,N_{k\neq j}} + \left(\frac{\partial A^{*,LR}}{\partial N_j}\right)_{T,V,N_{k\neq j}} + \left(\frac{\partial A^{*,LR}}{\partial V}\right)_{T,P,N_j}\left(\frac{\partial V}{\partial N_j}\right)_{T,P,N_{k\neq j}}\right)$$

A Novel, Tight Interval Extension Rule

$$f(\mathbf{x}) = \frac{\mathbf{x}^{\mathrm{T}} \exp(\mathbf{x})}{\mathbf{1}^{\mathrm{T}} \exp(\mathbf{x})} = \frac{x_1 \exp(x_1) + x_2 \exp(x_2) + \ldots + x_n \exp(x_n)}{\exp(x_1) + \exp(x_2) + \ldots + \exp(x_n)}$$

$$= \frac{x_1 \cancel{\exp(x_1)}}{\exp(x_1) + \exp(x_2) + \ldots + \exp(x_n)} + \frac{x_2 \exp(x_2)}{\exp(x_1) + \exp(x_2) + \ldots + \exp(x_n)} + \ldots + \frac{x_n \exp(x_n)}{\exp(x_1) + \exp(x_2) + \ldots + \exp(x_n)}$$

$$= \frac{x_1}{1 + \exp(x_2 - x_1) + \ldots + \exp(x_n - x_1)} + \frac{x_2}{\exp(x_1 - x_2) + 1 + \ldots + \exp(x_n - x_2)} + \ldots + \frac{x_n}{\exp(x_1 - x_n) + \exp(x_2 - x_n) + \ldots + 1}$$

$$= \sum_{i=1}^{n} \frac{x_i}{1 + \sum_{j=1, j \neq i}^{n} \exp(x_j - x_i)}$$

Challenge: Dependency Problem

Abstracted Form of Problematic Terms

$$\left(\frac{\sum_{j=1}^{n} \exp(x_j) x_j}{\sum_{j=1}^{n} \exp(x_j)} \right)$$

EX: 1 Term

$$x_j = [x_j^L, x_j^U] \longrightarrow \exp(x_j) \in [\exp(x_j^L), \exp(x_j^U)]$$

$$x_j \exp(x_j) \in \left[\min\left(x_j^L \exp(x_j^U), x_j^L \exp(x_j^L)\right), \max\left(x_j^U \exp(x_j^U), x_j^U \exp(x_j^L)\right)\right]$$

$$\frac{x_j \exp(x_j)}{\exp(x_j)} \in \left[\min\left\{\frac{x_j^L \exp(x_j^U)}{\exp(x_j^L)}, \frac{x_j^L \exp(x_j^L)}{\exp(x_j^L)}\right\}, \max\left\{\frac{x_j^U \exp(x_j^U)}{\exp(x_j^L)}, \frac{x_j^U \exp(x_j^L)}{\exp(x_j^L)}\right\}\right]$$