

On the Derivation of Continuous Piecewise Linear Approximating Functions

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S1. Alternative Formulation of Eq. (5)

First, we introduce a new continuous variable Y_i . Then, Eq. (5) is replaced by the following constraints:

$$Y_i \geq x_i A_k + B_k - \mu_i^L (1 - Z_{i,k}), i \in \mathbf{I}, k \in \mathbf{K}^I \quad (\text{S1.1})$$

$$Y_i \leq x_i A_k + B_k + \mu_i^U (1 - Z_{i,k}), i \in \mathbf{I}, k \in \mathbf{K}^I \quad (\text{S1.2})$$

In addition, Eqs. (6) and (7) must be modified:

$$E_i \geq Y_i - y_i, i \in \mathbf{I} \quad (\text{S1.3})$$

$$E_i \geq y_i - Y_i, i \in \mathbf{I} \quad (\text{S1.4})$$

S2. Reference System and Big-M Parameter Calculation

Without a loss of generality, we can adopt a reference system so that the shifted data points (\hat{x}_i, \hat{y}_i) will all be in the first quadrant:

$$\hat{x}_i = x_i - \min_{i'} x_{i'}, i \in \mathbf{I} \quad (\text{S2.1})$$

$$\hat{y}_i = y_i - \min_{i'} y_{i'}, i \in \mathbf{I} \quad (\text{S2.2})$$

We show that tight big-M parameters can be calculated based on a new reference system. This change of reference system can be applied even when the original data set is already in the first quadrant. Once the optimization model is solved using the shifted data, the optimal slope and intercept $(\hat{A}_k$ and $\hat{B}_k)$ can be post-processed to obtain the fitting function for the original data:

$$A_k = \hat{A}_k, k \in \mathbf{K}^I \quad (\text{S2.3})$$

$$B_k = \hat{B}_k + \min_i y_i - \hat{A}_k \min_i x_i, k \in \mathbf{K}^I \quad (\text{S2.4})$$

Therefore, when the shifted data set is used, μ_i^U and μ_i^L in Eqs. (6) and (7) can be calculated as follows:

$$\mu_i^U = \bar{A} \hat{x}_i + \bar{B} - \hat{y}_i, i \in \mathbf{I} \quad (\text{S2.5})$$

$$\mu_i^L = \hat{y}_i - \underline{A} \hat{x}_i - \underline{B}, i \in \mathbf{I} \quad (\text{S2.6})$$

where \bar{A} and \underline{A} are upper/lower bounds on slope, and \bar{B} and \underline{B} are bounds on intercept.

S3. Data Set in §4.1

Table S1. VLE data set

| i | x_i | y_i |
|-----|--------|--------|
| 1 | 0.0000 | 0.0000 |
| 2 | 0.0160 | 0.1470 |
| 3 | 0.0315 | 0.2505 |
| 4 | 0.0600 | 0.3765 |
| 5 | 0.0855 | 0.4300 |
| 6 | 0.1465 | 0.5005 |
| 7 | 0.2060 | 0.5415 |
| 8 | 0.2360 | 0.5600 |
| 9 | 0.3495 | 0.5945 |
| 10 | 0.4675 | 0.6410 |
| 11 | 0.4875 | 0.6425 |
| 12 | 0.5800 | 0.6890 |
| 13 | 0.6525 | 0.7250 |
| 14 | 0.7000 | 0.7495 |
| 15 | 0.7175 | 0.7680 |
| 16 | 0.7890 | 0.8111 |
| 17 | 0.8420 | 0.8488 |
| 18 | 0.8749 | 0.8768 |
| 19 | 0.8967 | 0.8973 |
| 20 | 0.9485 | 0.9440 |
| 21 | 0.9727 | 0.9692 |
| 22 | 1.0000 | 1.0000 |

S4. Data Sets in §4.2

Table S2. Data set in instance 1

| i | x_i | y_i |
|-----|--------|--------|
| 1 | 0.0000 | 0.0000 |
| 2 | 0.0196 | 0.0334 |
| 3 | 0.0392 | 0.0658 |
| 4 | 0.0588 | 0.0973 |
| 5 | 0.0784 | 0.1280 |
| 6 | 0.0980 | 0.1578 |
| 7 | 0.1176 | 0.1868 |
| 8 | 0.1373 | 0.2150 |
| 9 | 0.1569 | 0.2425 |
| 10 | 0.1765 | 0.2692 |
| 11 | 0.1961 | 0.2953 |
| 12 | 0.2157 | 0.3207 |
| 13 | 0.2353 | 0.3455 |
| 14 | 0.2549 | 0.3696 |
| 15 | 0.2745 | 0.3931 |
| 16 | 0.2941 | 0.4161 |
| 17 | 0.3137 | 0.4385 |
| 18 | 0.3333 | 0.4604 |
| 19 | 0.3529 | 0.4818 |
| 20 | 0.3725 | 0.5027 |
| 21 | 0.3922 | 0.5231 |
| 22 | 0.4118 | 0.5431 |
| 23 | 0.4314 | 0.5626 |
| 24 | 0.4510 | 0.5817 |
| 25 | 0.4706 | 0.6004 |
| 26 | 0.4902 | 0.6188 |
| 27 | 0.5098 | 0.6367 |
| 28 | 0.5294 | 0.6543 |
| 29 | 0.5490 | 0.6715 |
| 30 | 0.5686 | 0.6884 |
| 31 | 0.5882 | 0.7050 |
| 32 | 0.6078 | 0.7213 |
| 33 | 0.6275 | 0.7373 |
| 34 | 0.6471 | 0.7530 |
| 35 | 0.6667 | 0.7684 |
| 36 | 0.6863 | 0.7836 |
| 37 | 0.7059 | 0.7985 |
| 38 | 0.7255 | 0.8132 |
| 39 | 0.7451 | 0.8277 |
| 40 | 0.7647 | 0.8420 |
| 41 | 0.7843 | 0.8560 |

| | | |
|----|--------|--------|
| 42 | 0.8039 | 0.8699 |
| 43 | 0.8235 | 0.8836 |
| 44 | 0.8431 | 0.8971 |
| 45 | 0.8627 | 0.9104 |
| 46 | 0.8824 | 0.9236 |
| 47 | 0.9020 | 0.9366 |
| 48 | 0.9216 | 0.9495 |
| 49 | 0.9412 | 0.9623 |
| 50 | 0.9608 | 0.9750 |
| 51 | 0.9804 | 0.9875 |
| 52 | 1.0000 | 1.0000 |

Table S3. Data set in instance 2

| i | x_i | y_i |
|-----|--------|--------|
| 1 | 0.0000 | 0.0000 |
| 2 | 0.0196 | 0.1812 |
| 3 | 0.0392 | 0.2872 |
| 4 | 0.0588 | 0.3562 |
| 5 | 0.0784 | 0.4044 |
| 6 | 0.0980 | 0.4399 |
| 7 | 0.1176 | 0.4672 |
| 8 | 0.1373 | 0.4887 |
| 9 | 0.1569 | 0.5063 |
| 10 | 0.1765 | 0.5210 |
| 11 | 0.1961 | 0.5336 |
| 12 | 0.2157 | 0.5446 |
| 13 | 0.2353 | 0.5544 |
| 14 | 0.2549 | 0.5634 |
| 15 | 0.2745 | 0.5718 |
| 16 | 0.2941 | 0.5796 |
| 17 | 0.3137 | 0.5872 |
| 18 | 0.3333 | 0.5945 |
| 19 | 0.3529 | 0.6017 |
| 20 | 0.3725 | 0.6088 |
| 21 | 0.3922 | 0.6159 |
| 22 | 0.4118 | 0.6231 |
| 23 | 0.4314 | 0.6304 |
| 24 | 0.4510 | 0.6378 |
| 25 | 0.4706 | 0.6454 |
| 26 | 0.4902 | 0.6532 |
| 27 | 0.5098 | 0.6612 |
| 28 | 0.5294 | 0.6694 |
| 29 | 0.5490 | 0.6780 |
| 30 | 0.5686 | 0.6868 |

| | | |
|----|--------|--------|
| 31 | 0.5882 | 0.6959 |
| 32 | 0.6078 | 0.7053 |
| 33 | 0.6275 | 0.7151 |
| 34 | 0.6471 | 0.7253 |
| 35 | 0.6667 | 0.7359 |
| 36 | 0.6863 | 0.7468 |
| 37 | 0.7059 | 0.7582 |
| 38 | 0.7255 | 0.7701 |
| 39 | 0.7451 | 0.7825 |
| 40 | 0.7647 | 0.7953 |
| 41 | 0.7843 | 0.8087 |
| 42 | 0.8039 | 0.8226 |
| 43 | 0.8235 | 0.8371 |
| 44 | 0.8431 | 0.8523 |
| 45 | 0.8627 | 0.8681 |
| 46 | 0.8824 | 0.8845 |
| 47 | 0.9017 | 0.9017 |

S5. Details of Computational Studies in §4.3

Table S4. Specifications and solution statistics for the computational studies

| instance | description | # data points | # breaks | solution time (sec) | | |
|----------|------------------------------------|---------------|----------|---------------------|-------|-------|
| | | | | M1 | M1* | M0 |
| 1 | | | 4 | 0.63 | 1.28 | 8.70 |
| 2 | ethanol-water VLE | 22 | 5 | 1.81 | 4.13 | 435 |
| 3 | | | 6 | 2.27 | 7.30 | 1800* |
| 4 | | | 7 | 10.0 | 19.6 | 1800* |
| 5 | water heat capacity | 26 | 4 | 1.92 | 2.13 | 33.8 |
| 6 | | | 6 | 8.30 | 11.5 | 308 |
| 7 | | | 7 | 12.5 | 74.6 | 1800* |
| 8 | world population | 57 | 4 | 66.0 | 54.5 | 1800* |
| 9 | | | 5 | 147 | 206 | 1800* |
| 10 | | | 6 | 264 | 270 | 1800* |
| 11 | ASPEN simulation | 15 | 4 | 0.34 | 0.66 | 12.0 |
| 12 | | | 5 | 1.14 | 0.95 | 101 |
| 13 | | | 6 | 2.69 | 1.58 | 320 |
| 14 | steam compressibility factor | 100 | 4 | 9.4 | 158 | 43.6 |
| 15 | | | 5 | 162 | 510 | 1280 |
| 16 | | | 6 | 1593 | 1800* | 1800* |
| 17 | | | 7 | 1800* | 1800* | 1800* |

The optimization problem cannot be solved to optimality within the 1800 sec time limit; M1 utilizes tight bounds and big-M; M1 uses 1000 for all the big-M parameters and does not specify bounds on A_k or B_k .

Table S5. Comparison of global optimization solvers

| instance | description | # breaks | solution time (sec) or optimality gap | | |
|----------|------------------------------------|----------|--|-------------|------------|
| | | | ANTIGONE | BARON | SCIP |
| 1 | | 4 | 0.16% | 8.7 | 29 |
| 2 | ethanol-water VLE | 5 | 0.55% | 435 | Inf |
| 3 | | 6 | 1.25% | 642 | Inf |
| 4 | | 7 | 40.3% | 96.3% | Inf |
| 5 | | 4 | 0.0003% | 33.8 | Inf |
| 6 | water heat capacity | 6 | 0.009% | 308 | Inf |
| 7 | | 7 | 3.68% | Inf | Inf |
| 8 | | 4 | 30.6% | Inf | Inf |
| 9 | world population | 5 | 84.1% | Inf | Inf |
| 10 | | 6 | 99.9% | Inf | Inf |
| 11 | | 4 | 0.002% | 39 | 12 |
| 12 | ASPEN simulation | 5 | 917 | 170 | 101 |
| 13 | | 6 | 2.02% | 433 | 320 |
| 14 | | 4 | 257 | 43.6 | Inf |
| 15 | steam compressibility factor | 5 | 0.01% | 1276 | Inf |
| 16 | | 6 | 63.2% | Inf | Inf |
| 17 | | 7 | Inf | Inf | Inf |

Entries with "Inf" means the solver did not find a positive lower bound (i.e. infinity gap)

Table S6. Ethanol-water VLE

| i | x_i | y_i |
|-----|--------|--------|
| 1 | 0.0000 | 0.0000 |
| 2 | 0.0160 | 0.1470 |
| 3 | 0.0315 | 0.2505 |
| 4 | 0.0600 | 0.3765 |
| 5 | 0.0855 | 0.4300 |
| 6 | 0.1465 | 0.5005 |
| 7 | 0.2060 | 0.5415 |
| 8 | 0.2360 | 0.5600 |
| 9 | 0.3495 | 0.5945 |
| 10 | 0.4675 | 0.6410 |
| 11 | 0.4875 | 0.6425 |
| 12 | 0.5800 | 0.6890 |
| 13 | 0.6525 | 0.7250 |
| 14 | 0.7000 | 0.7495 |
| 15 | 0.7175 | 0.7680 |
| 16 | 0.7890 | 0.8111 |
| 17 | 0.8420 | 0.8488 |
| 18 | 0.8749 | 0.8768 |
| 19 | 0.8967 | 0.8973 |
| 20 | 0.9485 | 0.9440 |
| 21 | 0.9727 | 0.9692 |
| 22 | 1.0000 | 1.0000 |

Beebe, A.H.; Coulter, K.E.; Lindsay, R.A.; Baker, E.M.: Equilibria in Ethanol-Water System at Pressures Less Than Atmospheric. *Ind.Eng.Chem. Ind.Ed.* 34 (1942) 1501-1504

Table S7. Water heat capacity

| i | x_i | y_i |
|-----|-------|--------|
| 1 | 0.01 | 75.981 |
| 2 | 10 | 75.505 |
| 3 | 20 | 74.893 |
| 4 | 25 | 74.548 |
| 5 | 30 | 74.181 |
| 6 | 40 | 73.392 |
| 7 | 50 | 72.540 |
| 8 | 60 | 71.644 |
| 9 | 70 | 70.716 |
| 10 | 80 | 69.774 |
| 11 | 90 | 68.828 |
| 12 | 100 | 67.888 |
| 13 | 110 | 66.960 |
| 14 | 120 | 66.050 |
| 15 | 140 | 64.306 |
| 16 | 160 | 62.674 |
| 17 | 180 | 61.163 |
| 18 | 200 | 59.775 |
| 19 | 220 | 58.514 |
| 20 | 240 | 57.381 |
| 21 | 260 | 56.392 |
| 22 | 280 | 55.578 |
| 23 | 300 | 55.003 |
| 24 | 320 | 54.819 |
| 25 | 340 | 55.455 |
| 26 | 360 | 59.402 |

Engineering ToolBox, (2004). *Water - Heat Capacity (Specific Heat)* . [online] Available at: https://www.engineeringtoolbox.com/specific-heat-capacity-water-d_660.html [Accessed 5/14/2018]

Table S8. Percent of female population ages 25-29 from year 1960 to 2016

| i | x_i | y_i |
|-----|-------|----------|
| 1 | 1.960 | 0.00196 |
| 2 | 1.961 | 0.001961 |
| 3 | 1.962 | 0.001962 |
| 4 | 1.963 | 0.001963 |
| 5 | 1.964 | 0.001964 |
| 6 | 1.965 | 0.001965 |
| 7 | 1.966 | 0.001966 |
| 8 | 1.967 | 0.001967 |
| 9 | 1.968 | 0.001968 |
| 10 | 1.969 | 0.001969 |
| 11 | 1.970 | 0.001970 |
| 12 | 1.971 | 0.001971 |
| 13 | 1.972 | 0.001972 |
| 14 | 1.973 | 0.001973 |
| 15 | 1.974 | 0.001974 |
| 16 | 1.975 | 0.001975 |
| 17 | 1.976 | 0.001976 |
| 18 | 1.977 | 0.001977 |
| 19 | 1.978 | 0.001978 |
| 20 | 1.979 | 0.001979 |
| 21 | 1.980 | 0.001980 |
| 22 | 1.981 | 0.001981 |
| 23 | 1.982 | 0.001982 |
| 24 | 1.983 | 0.001983 |
| 25 | 1.984 | 0.001984 |
| 26 | 1.985 | 0.001985 |
| 27 | 1.986 | 0.001986 |
| 28 | 1.987 | 0.001987 |
| 29 | 1.988 | 0.001988 |
| 30 | 1.989 | 0.001989 |
| 31 | 1.990 | 0.001990 |
| 32 | 1.991 | 0.001991 |
| 33 | 1.992 | 0.001992 |
| 34 | 1.993 | 0.001993 |
| 35 | 1.994 | 0.001994 |
| 36 | 1.995 | 0.001995 |
| 37 | 1.996 | 0.001996 |
| 38 | 1.997 | 0.001997 |
| 39 | 1.998 | 0.001998 |
| 40 | 1.999 | 0.001999 |
| 41 | 2.000 | 0.002000 |

| | | |
|----|-------|----------|
| 42 | 2.001 | 0.002001 |
| 43 | 2.002 | 0.002002 |
| 44 | 2.003 | 0.002003 |
| 45 | 2.004 | 0.002004 |
| 46 | 2.005 | 0.002005 |
| 47 | 2.006 | 0.002006 |
| 48 | 2.007 | 0.002007 |
| 49 | 2.008 | 0.002008 |
| 50 | 2.009 | 0.002009 |
| 51 | 2.010 | 0.002010 |
| 52 | 2.011 | 0.002011 |
| 53 | 2.012 | 0.002012 |
| 54 | 2.013 | 0.002013 |
| 55 | 2.014 | 0.002014 |
| 56 | 2.015 | 0.002015 |
| 57 | 2.016 | 0.002016 |

<https://data.worldbank.org/indicator/SP.POP.2529.FE.5Y?end=2016&start=1960> [Accessed 5/14/2018]

Table S9. ASPEN simulation

| i | x_i | y_i |
|-----|----------|----------|
| 1 | 0.859905 | 12.43300 |
| 2 | 0.899905 | 13.74640 |
| 3 | 0.909904 | 14.18700 |
| 4 | 0.919904 | 14.69294 |
| 5 | 0.929902 | 15.28137 |
| 6 | 0.939963 | 15.98235 |
| 7 | 0.949984 | 16.65584 |
| 8 | 0.959999 | 17.21400 |
| 9 | 0.969915 | 17.93359 |
| 10 | 0.979912 | 18.95811 |
| 11 | 0.989995 | 20.72504 |
| 12 | 0.992380 | 21.41773 |
| 13 | 0.994993 | 22.49604 |
| 14 | 0.998999 | 26.82566 |
| 15 | 0.999500 | 28.77289 |

Kong, L., et al. "A superstructure-based framework for simultaneous process synthesis, heat integration, and utility plant design." *Computers & Chemical Engineering* 91 (2016): 68-84.

Table S10. Steam compressibility factor

| i | x_i | y_i |
|-----|-------|----------|
| 1 | 0.01 | 8.667502 |
| 2 | 0.02 | 4.336951 |
| 3 | 0.03 | 2.894065 |
| 4 | 0.04 | 2.173009 |
| 5 | 0.05 | 1.740645 |
| 6 | 0.06 | 1.452605 |
| 7 | 0.07 | 1.247024 |
| 8 | 0.08 | 1.092971 |
| 9 | 0.09 | 0.973264 |
| 10 | 0.10 | 0.877596 |
| 11 | 0.11 | 0.799407 |
| 12 | 0.12 | 0.734326 |
| 13 | 0.13 | 0.679326 |
| 14 | 0.14 | 0.632246 |
| 15 | 0.15 | 0.591501 |
| 16 | 0.16 | 0.555903 |
| 17 | 0.17 | 0.524543 |
| 18 | 0.18 | 0.496715 |
| 19 | 0.19 | 0.471861 |
| 20 | 0.20 | 0.449535 |
| 21 | 0.21 | 0.429375 |
| 22 | 0.22 | 0.411087 |
| 23 | 0.23 | 0.394427 |
| 24 | 0.24 | 0.379191 |
| 25 | 0.25 | 0.365209 |
| 26 | 0.26 | 0.352336 |
| 27 | 0.27 | 0.340450 |
| 28 | 0.28 | 0.329446 |
| 29 | 0.29 | 0.319232 |
| 30 | 0.30 | 0.309731 |
| 31 | 0.31 | 0.300873 |
| 32 | 0.32 | 0.292599 |
| 33 | 0.33 | 0.284856 |
| 34 | 0.34 | 0.277599 |
| 35 | 0.35 | 0.270785 |
| 36 | 0.36 | 0.264380 |
| 37 | 0.37 | 0.258350 |
| 38 | 0.38 | 0.252666 |
| 39 | 0.39 | 0.247303 |
| 40 | 0.40 | 0.242237 |
| 41 | 0.41 | 0.237447 |

| | | |
|----|------|----------|
| 42 | 0.42 | 0.232915 |
| 43 | 0.43 | 0.228623 |
| 44 | 0.44 | 0.224555 |
| 45 | 0.45 | 0.220698 |
| 46 | 0.46 | 0.217039 |
| 47 | 0.47 | 0.213566 |
| 48 | 0.48 | 0.210269 |
| 49 | 0.49 | 0.207138 |
| 50 | 0.50 | 0.204163 |
| 51 | 0.51 | 0.201338 |
| 52 | 0.52 | 0.198654 |
| 53 | 0.53 | 0.196104 |
| 54 | 0.54 | 0.193684 |
| 55 | 0.55 | 0.191386 |
| 56 | 0.56 | 0.189206 |
| 57 | 0.57 | 0.187139 |
| 58 | 0.58 | 0.185181 |
| 59 | 0.59 | 0.183328 |
| 60 | 0.60 | 0.181576 |
| 61 | 0.61 | 0.179923 |
| 62 | 0.62 | 0.178365 |
| 63 | 0.63 | 0.176901 |
| 64 | 0.64 | 0.175528 |
| 65 | 0.65 | 0.174244 |
| 66 | 0.66 | 0.173047 |
| 67 | 0.67 | 0.171939 |
| 68 | 0.68 | 0.170915 |
| 69 | 0.69 | 0.169977 |
| 70 | 0.70 | 0.169124 |
| 71 | 0.71 | 0.168356 |
| 72 | 0.72 | 0.167674 |
| 73 | 0.73 | 0.167078 |
| 74 | 0.74 | 0.166571 |
| 75 | 0.75 | 0.166153 |
| 76 | 0.76 | 0.165828 |
| 77 | 0.77 | 0.165598 |
| 78 | 0.78 | 0.165467 |
| 79 | 0.79 | 0.165439 |
| 80 | 0.80 | 0.165519 |
| 81 | 0.81 | 0.165715 |
| 82 | 0.82 | 0.166033 |
| 83 | 0.83 | 0.166484 |
| 84 | 0.84 | 0.167075 |

| | | |
|-----|------|----------|
| 85 | 0.85 | 0.167827 |
| 86 | 0.86 | 0.168749 |
| 87 | 0.87 | 0.169852 |
| 88 | 0.88 | 0.171202 |
| 89 | 0.89 | 0.172788 |
| 90 | 0.90 | 0.174664 |
| 91 | 0.91 | 0.176875 |
| 92 | 0.92 | 0.179530 |
| 93 | 0.93 | 0.182687 |
| 94 | 0.94 | 0.186479 |
| 95 | 0.95 | 0.191183 |
| 96 | 0.96 | 0.197123 |
| 97 | 0.97 | 0.204893 |
| 98 | 0.98 | 0.215925 |
| 99 | 0.99 | 0.234045 |
| 100 | 1.00 | 0.372727 |

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