Uncertainty and Variability Modeling via Data-Driven Chance Constraints

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Modeling Uncertainty in Optimization

- Optimization models for real-world applications are expected to generate "robust" decisions in the face of uncertainty.
- Models use historical and predicted data subject to uncertainty.
- Examples of data variability and uncertainty:
  - Product demand and selling price;
  - Raw material supply;
  - Production rates etc.
- Some approaches of optimization under uncertainty:
  - Stochastic Programming (Birge & Louveaux, 2011);
  - Robust Optimization (Ben-Tal, Ghaoui, & Nemirovski, 2009);
  - Approximate Dynamic Programming (Powell, 2011) etc.
- **This work:** Chance-Constrained Optimization (Charnes & Cooper, 1959).

Chance-Constrained Optimization

- Chance constrains (CCs) are also known as probabilistic constraints.
- Optimization model with joint chance constraint (JCC)

$$\max_x \ f(x)$$
$$\text{s.t.} \quad x \in X$$
$$\mathbb{P}\left\{g_j(x, \tilde{\xi}_j) \geq 0,\ j = 1,\ \ldots,\ m\right\} \geq 1 - \alpha$$

- Optimization model with individual (or disjoint) chance constraint (ICC)

$$\max_x \ f(x)$$
$$\text{s.t.} \quad x \in X$$
$$\mathbb{P}\left\{g_j(x, \tilde{\xi}_j) \geq 0\right\} \geq 1 - \alpha_j \qquad j = 1,\ \ldots,\ m$$

where $X \subset \mathbb{R}^{n_x}$ determines the feasible region (e.g., polyhedron)

- **This work:** right-hand side (RHS) uncertainty only.

Classical Chance Constraints

- CCs with RHS uncertainty are very common in engineering applications
  - Chemical Engineering: maximum production rates, demand satisfaction, setpoint tracking in dynamic optimization
  - Electrical Engineering: power supply for demand satisfaction
  - Hydrology: reservoir storage levels (water availability)
- The general chance constraints

$$\mathbb{P}\left\{g_j(x) \geq \tilde{\xi}_j\right\} \geq 1 - \alpha_j, \qquad j = 1, \ldots, m \quad \text{(ICC)}$$

$$\mathbb{P}\left\{g_j(x) \geq \tilde{\xi}_j,\ j = 1, \ldots, m\right\} \geq 1 - \alpha \quad \text{(JCC)}$$

can be reformulated as follows

$$g_j(x) \geq F_{\xi_j}^{-1}(1 - \alpha_j), \qquad \text{for } j = 1, \ldots, m \quad \text{(ICC)}$$

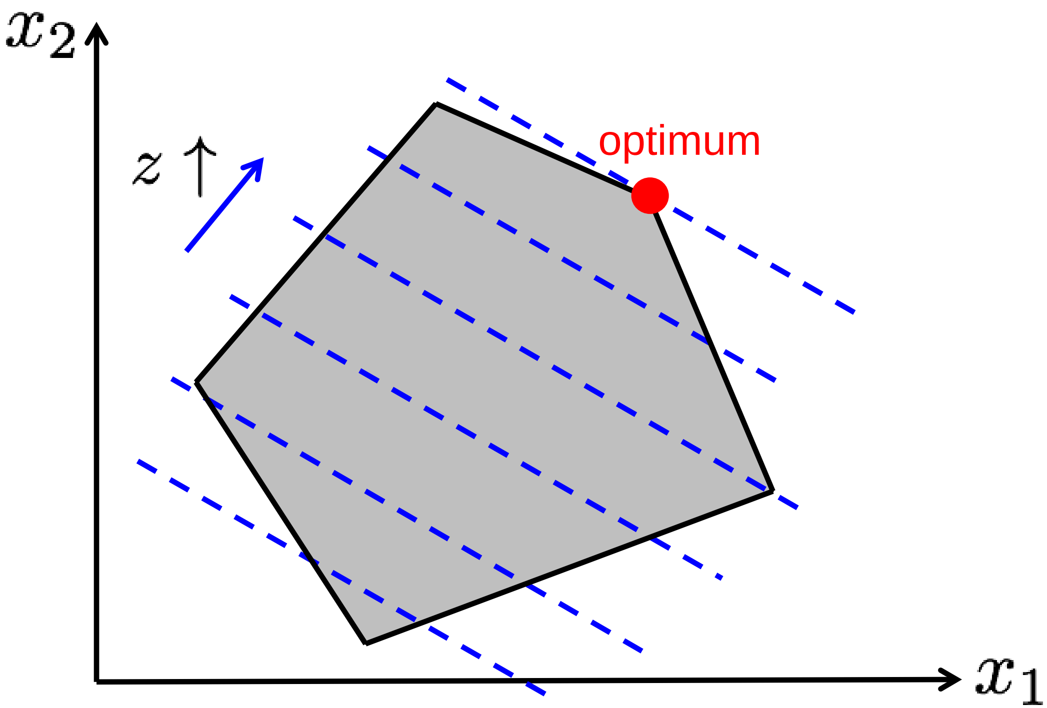
$$F_{\tilde{\xi}_{j=1}^{m}}(g_j(x), \ldots, g_m(x)) \geq 1 - \alpha \quad \text{(JCC)}$$

where $F_{\xi_j}^{-1}(\cdot)$ is the inverse (univariate) CDF (or quantile function) and $F_{\tilde{\xi}_{j=1}^{m}}(\cdot, \ldots, \cdot)$ is the (multivariate) joint CDF.

Illustration: Deterministic Model

- For simplicity, consider an LP model in two dimensions

$$\begin{aligned} \max_{x_1, x_2} \quad & z = c_1 x_1 + c_2 x_2 \\ \text{s.t.} \quad & A_{i,1} x_1 + A_{i,2} x_2 \leq b_i \\ & \qquad \forall\, i = 1, \ldots, 5 \\ & x_1,\ x_2 \geq 0 \end{aligned}$$



Individual Chance-Constrained Model

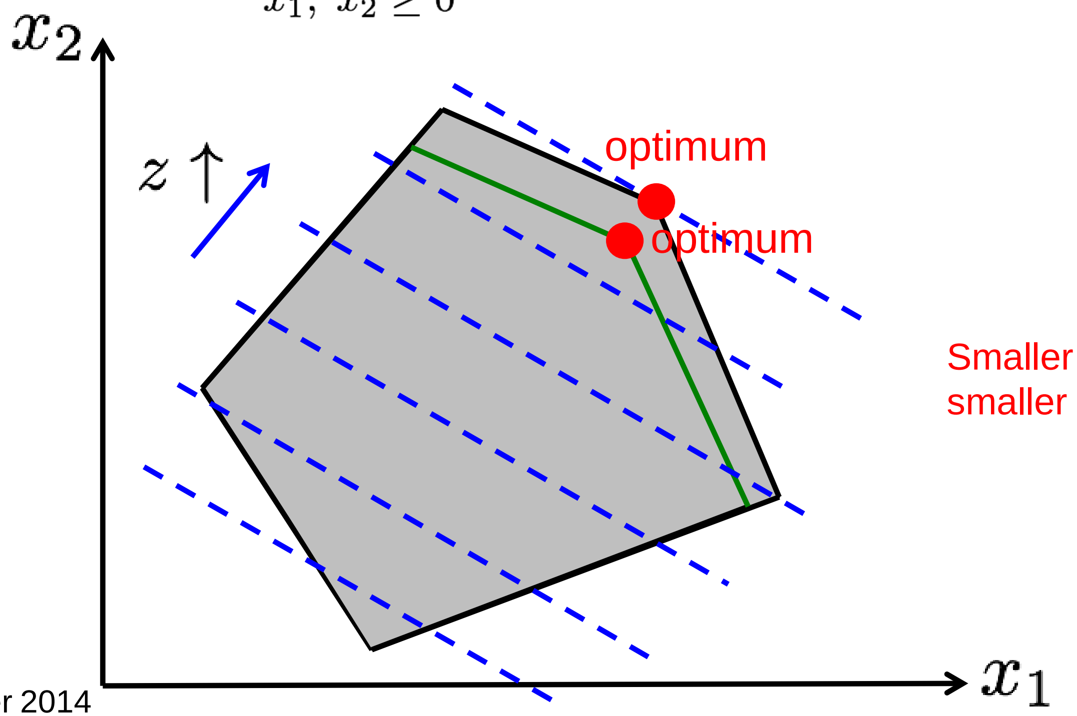
- Individual chance constraints (model remains an LP)

$$\max_{x_1, x_2} \; z = c_1 x_1 + c_2 x_2$$

$$\text{s.t.} \quad A_{i,1} x_1 + A_{i,2} x_2 \leq b_i \quad \forall\, i = 1,\ 2,\ 3$$

$$\mathbb{P}\left\{ A_{i,1} x_1 + A_{i,2} x_2 \leq \tilde{b}_i \right\} \geq 1 - \alpha_i \quad \forall\, i = 4,\ 5$$

$$x_1,\ x_2 \geq 0$$



Smaller feasible region for smaller risk level (α)

Individual Chance-Constrained Model

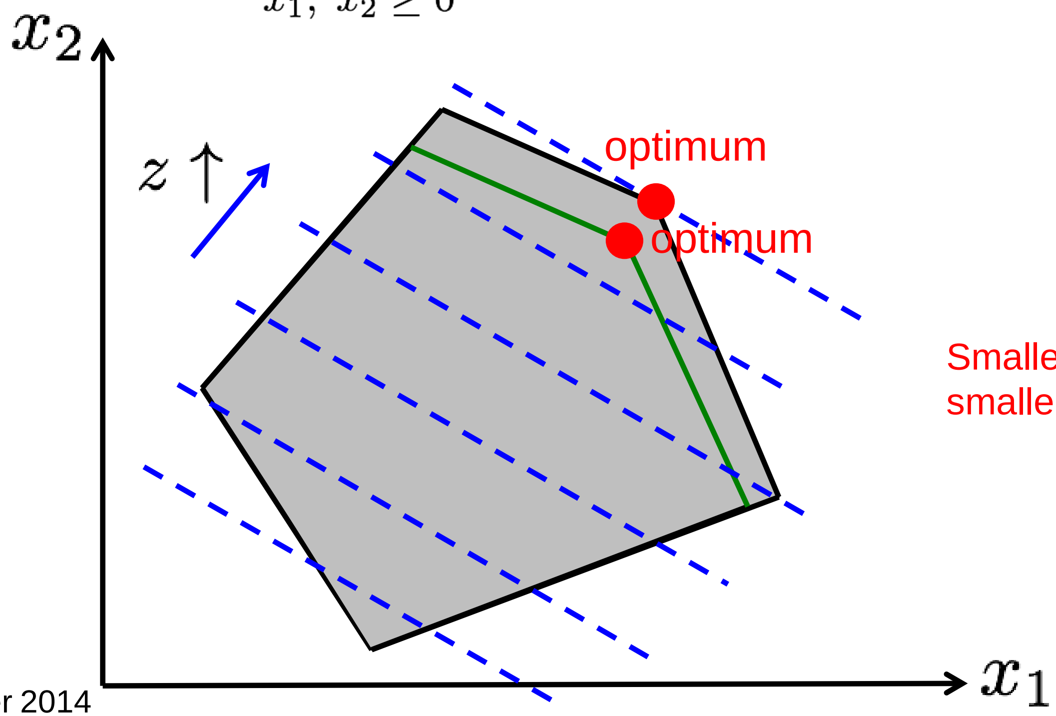
- Individual chance constraints (model remains an LP)

$$\max_{x_1,x_2} \; z = c_1 x_1 + c_2 x_2$$

$$\text{s.t.} \quad A_{i,1}x_1 + A_{i,2}x_2 \le b_i \quad \forall\, i = 1,\ 2,\ 3$$

$$A_{i,1}x_1 + A_{i,2}x_2 \le F_{\tilde{b}_i}^{-1}(\alpha_i) \quad \forall\, i = 4,\ 5$$

$$x_1,\ x_2 \ge 0$$



Smaller feasible region for smaller risk level (α)

Joint Chance-Constrained Model

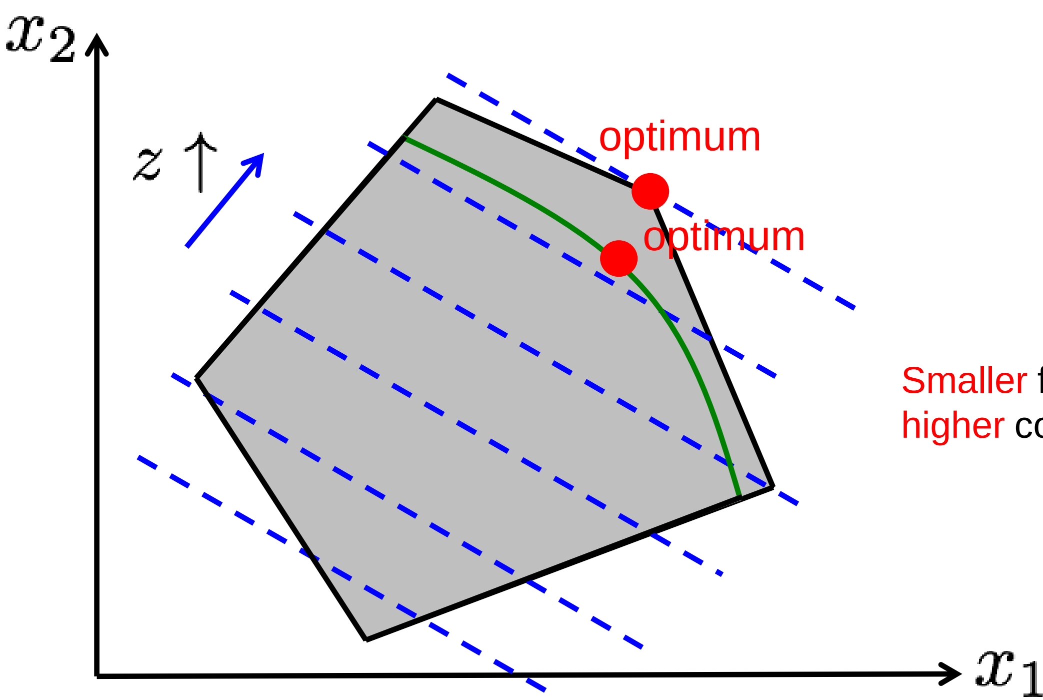
- Joint chance constraints (model is an NLP)

$$\max_{x_1,x_2} \; z = c_1x_1 + c_2x_2$$

$$\text{s.t.} \quad A_{i,1}x_1 + A_{i,2}x_2 \le b_i \qquad \forall\, i = 1,\ 2,\ 3$$

$$\mathbb{P}\left\{A_{i,1}x_1 + A_{i,2}x_2 \le \tilde{b}_i,\ \ i = 4, 5\right\} \ge 1 - \alpha$$

$$x_1,\ x_2 \ge 0$$



Smaller feasible region for higher confidence level $(1 - \alpha)$

Joint Chance-Constrained Model

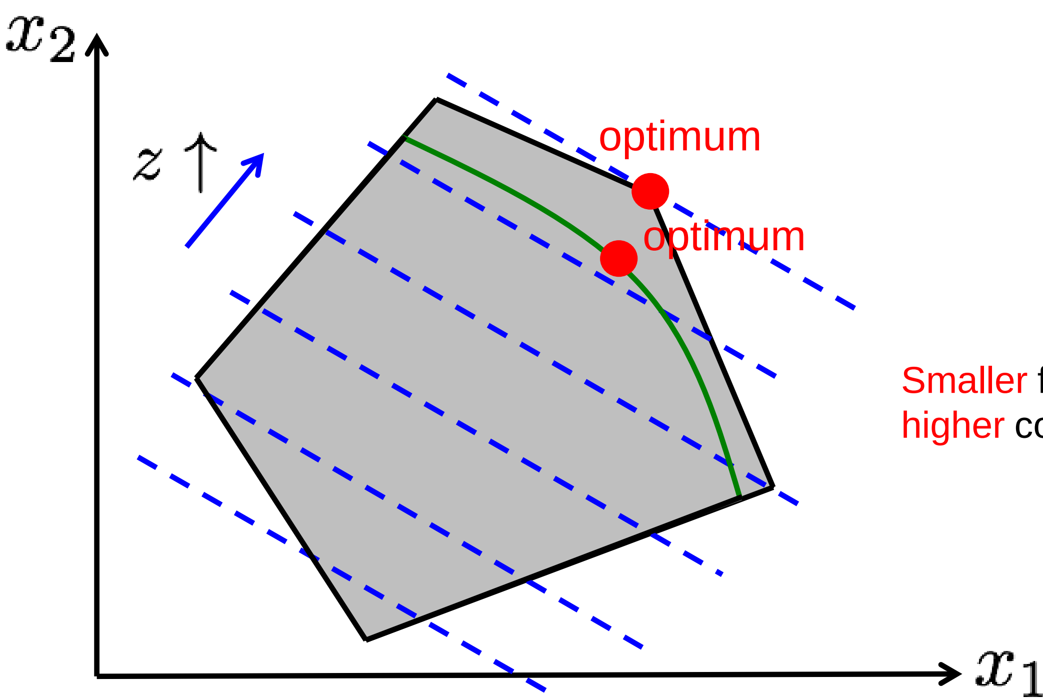
- Joint chance constraints (model is an NLP)

$$\max_{x_1, x_2} \; z = c_1 x_1 + c_2 x_2$$

$$\text{s.t.} \quad A_{i,1} x_1 + A_{i,2} x_2 \leq b_i \qquad \forall\, i = 1,\ 2,\ 3$$

$$\int_{A_{4,1}x_1 + A_{4,2}x_2}^{\infty} \int_{A_{5,1}x_1 + A_{5,2}x_2}^{\infty} f_{\tilde{b}_4, \tilde{b}_5}(b_4, b_5)\,\mathrm{d}b_4 \mathrm{d}b_5 \geq 1 - \alpha$$

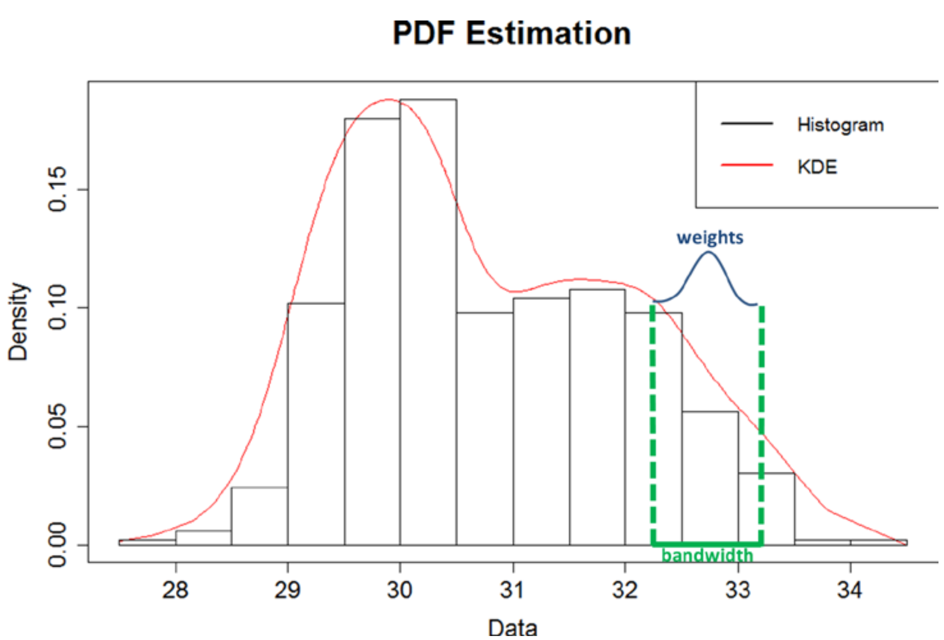
$$x_1,\ x_2 \geq 0$$



Smaller feasible region for higher confidence level (1 − α)

Data-Driven Chance-Constrained Optimization

- Very often in reality, distribution function is unknown or ambiguous.
- Nonparametric techniques: weaker model assumptions.
- Main result (Jiang and Guan, 2013)
  - Replace assumed "true" distribution $\mathbb{P}$ with its estimate $\hat{\mathbb{P}}$.
  - Risk level α is decreased to α'.



Kernel Density Estimation (KDE)

- Given i.i.d. data
- Estimate the PDF/CDF with a smooth curve
- Can estimate quantiles
- Decisions
  - Kernel function (typically Gaussian)
  - Bandwidth (optimization and cross-validation)
- Rigorous routines in R np package (Hayfield and Racine, 2008)

KDE Formulas

- Mathematical expressions for the univariate case (1-D):

PDF: $$\hat{f}(x) = \frac{1}{n}\sum_{i=1}^{n} K_h(x - x_i) = \frac{1}{nh}\sum_{i=1}^{n} K\left(\frac{x - x_i}{h}\right)$$

CDF: $$\hat{F}(x) = \frac{1}{n}\sum_{i=1}^{n} \mathcal{K}_h(x - x_i) = \frac{1}{n}\sum_{i=1}^{n} \mathcal{K}\left(\frac{x - x_i}{h}\right)$$

where $\mathcal{K}(\cdot)$ is the integrated kernel

- For multivariate, use *product kernels* (standard technique):

PDF: $$\hat{f}(x_1, \ldots, x_m) = \frac{1}{n}\sum_{i=1}^{n}\prod_{j=1}^{m} K_{h,j}(x_j - x_{i,j}) = \frac{1}{n}\sum_{i=1}^{n}\prod_{j=1}^{m} \frac{1}{h_j} K_j\left(\frac{x_j - x_{i,j}}{h_j}\right)$$

CDF: $$\hat{F}(x_1, \ldots, x_m) = \frac{1}{n}\sum_{i=1}^{n}\prod_{j=1}^{m} \mathcal{K}_{h,j}(x_j - x_{i,j}) = \frac{1}{n}\sum_{i=1}^{n}\prod_{j=1}^{m} \mathcal{K}_j\left(\frac{x_j - x_{i,j}}{h_j}\right)$$

- If using Gaussian kernel, then

$$K(u) = \phi(u) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}u^2} \qquad \mathcal{K}(u) = \Phi(u) = \frac{1}{2}\left[1 + \text{erf}\left(\frac{u}{\sqrt{2}}\right)\right]$$

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Kernel-Based Reformulation

- Original reformulated CCs:

$$g_j(x) \geq F_{\xi_j}^{-1}(1-\alpha_j), \qquad j = 1, \ldots, m \qquad \text{(ICC)}$$

$$F_{\tilde{\xi}_{j=1}^m}(g_1(x), \ldots, g_m(x)) \geq 1-\alpha \qquad \text{(JCC)}$$

- Kernel-based reformulation:

$$g_j(x) \geq \hat{F}_{\xi_j}^{-1}(1-\alpha'_{j,+}), \qquad j = 1, \ldots, m \qquad \text{(ICC)}$$

$$\hat{F}_{\tilde{\xi}_{j=1}^m}(g_1(x), \ldots, g_m(x)) \geq 1-\alpha'_+ \qquad \text{(JCC)}$$

or

$$\frac{1}{n}\sum_{i=1}^{n}\prod_{j=1}^{m}\mathcal{K}_j\left(\frac{g_j(x)-x_{i,j}}{h_j}\right) \geq 1-\alpha'_+ \qquad \text{(JCC)}$$

where α' is the decreased risk level due to the estimation process.

- **This work's contribution:** use of point-wise standard errors of the KDE process to compute α' using ϕ-divergences.

Calculating ϕ-Divergence Tolerance

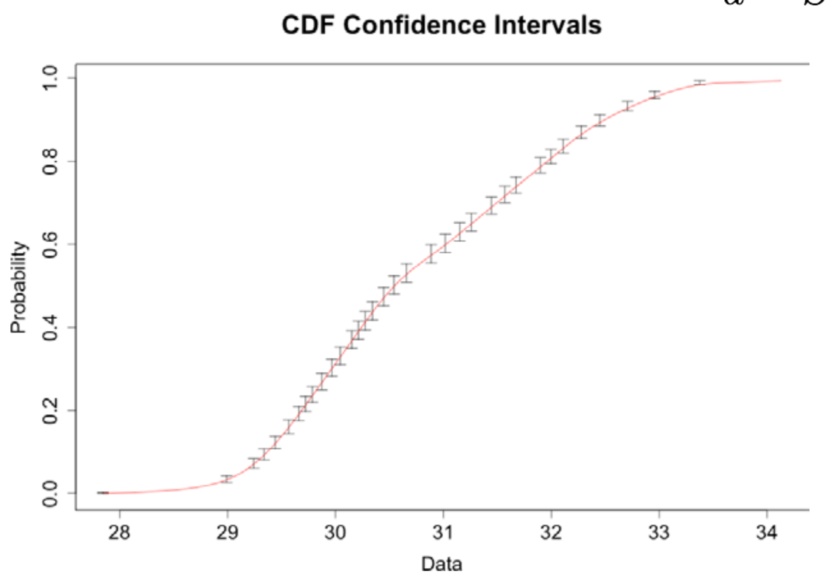
- Density-based confidence set and ϕ-divergence (distance between distributions):

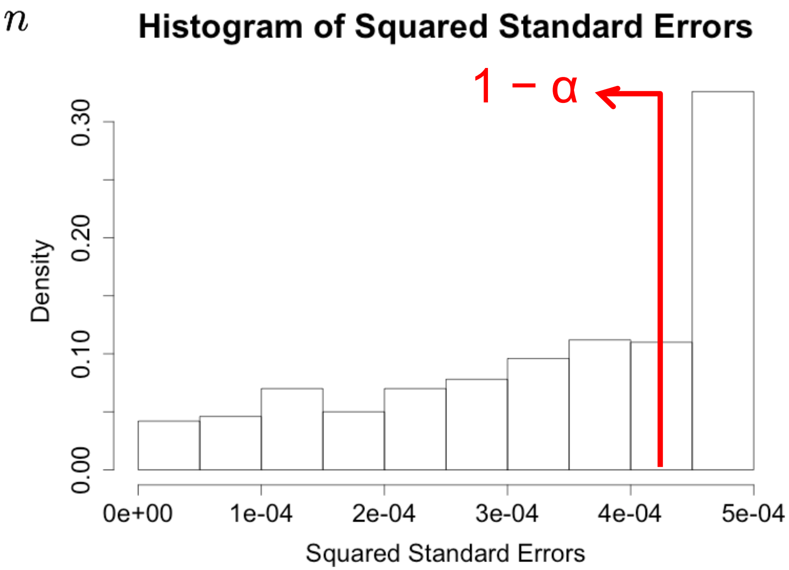
$$\mathcal{D} = \left\{ \mathbb{P} \in \mathcal{M}_+ : \; D_\phi(f||\hat{f}) \leq d \;\; f = \mathrm{d}\mathbb{P}/\mathrm{d}\tilde{\xi} \right\} \qquad D_\phi(f||\hat{f}) = \int_{\mathbb{R}^m} \phi\left(\frac{f(\tilde{\xi})}{\hat{f}(\tilde{\xi})}\right) \hat{f}(\tilde{\xi})\mathrm{d}\tilde{\xi}$$

e.g., Kullback-Leibler (K-L) divergence, $\phi(t) = t\log t - t + 1$.

- Proposed approach for calculating the divergence tolerance *d*
  - Square of point-wise standard errors from the quantile/distribution estimation via KDE. Bootstrapping or formulas based on the asymptotic normality of kernel estimators.

$$d = SE^2_{1-\alpha} \propto \frac{1}{n}$$

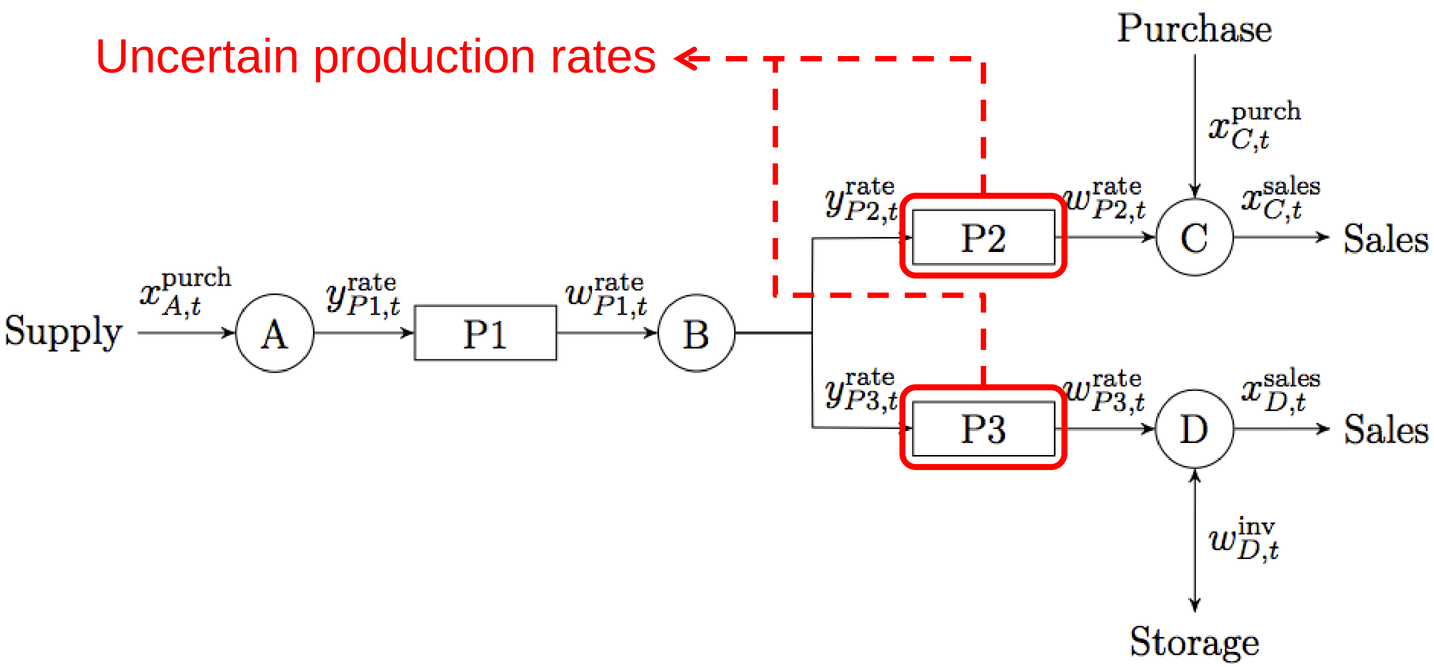




(Ben-Tal *et al.*, 2011; Jiang and Guan, 2013)

Motivating Example

- Network of chemical plants



- 1 raw material (A), 1 intermediate product (B), two finished products (C and D), 1 site
- Only D can be stored and C can be purchased from elsewhere (may simulate inter-site transfers)

Modeling Chance Constraints

- Uncertain production rates of plants *P2* and *P3*.
- ICC approach yields and LP (PPICC):

$$\mathbb{P}\left\{w^{\text{rate}}_{P2,t} \leq \tilde{\mathrm{w}}^{\text{rate,max}}_{P2}\right\} \geq 1-\alpha_{P2} \qquad \forall\, t \in T$$
$$\mathbb{P}\left\{w^{\text{rate}}_{P3,t} \leq \tilde{\mathrm{w}}^{\text{rate,max}}_{P3}\right\} \geq 1-\alpha_{P3} \qquad \forall\, t \in T$$

$$w^{\text{rate}}_{P2,t} \leq \hat{F}^{-1}_{\tilde{\mathrm{w}}^{\text{rate,max}}_{P2}}(\alpha'_{P2,+}) \qquad \forall\, t \in T$$
$$w^{\text{rate}}_{P3,t} \leq \hat{F}^{-1}_{\tilde{\mathrm{w}}^{\text{rate,max}}_{P3}}(\alpha'_{P3,+}) \qquad \forall\, t \in T$$

- JCC approach yields an NLP (PPJCC):

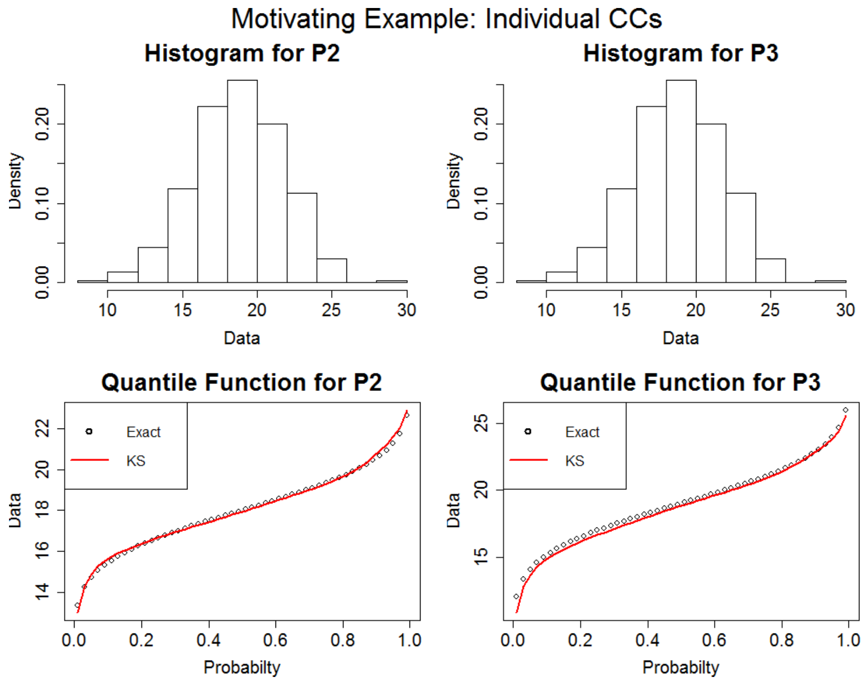
$$\mathbb{P}\left\{\begin{matrix} w^{\text{rate}}_{P2,t} \leq \tilde{\mathrm{w}}^{\text{rate,max}}_{P2} \\ w^{\text{rate}}_{P3,t} \leq \tilde{\mathrm{w}}^{\text{rate,max}}_{P3} \end{matrix}\right\} \geq 1-\alpha \qquad \forall\, t \in T$$

$$\frac{1}{n}\sum_{i=1}^{n}\left[1-\mathcal{K}_{P2}\left(\frac{w^{\text{rate}}_{P2,t}-\mathrm{w}^{\text{rate,max}}_{P2,i}}{h_{P2}}\right)\right]\left[1-\mathcal{K}_{P3}\left(\frac{w^{\text{rate}}_{P3,t}-\mathrm{w}^{\text{rate,max}}_{P3,i}}{h_{P3}}\right)\right] \geq 1-\alpha'_{+} \qquad \forall\, t \in T$$

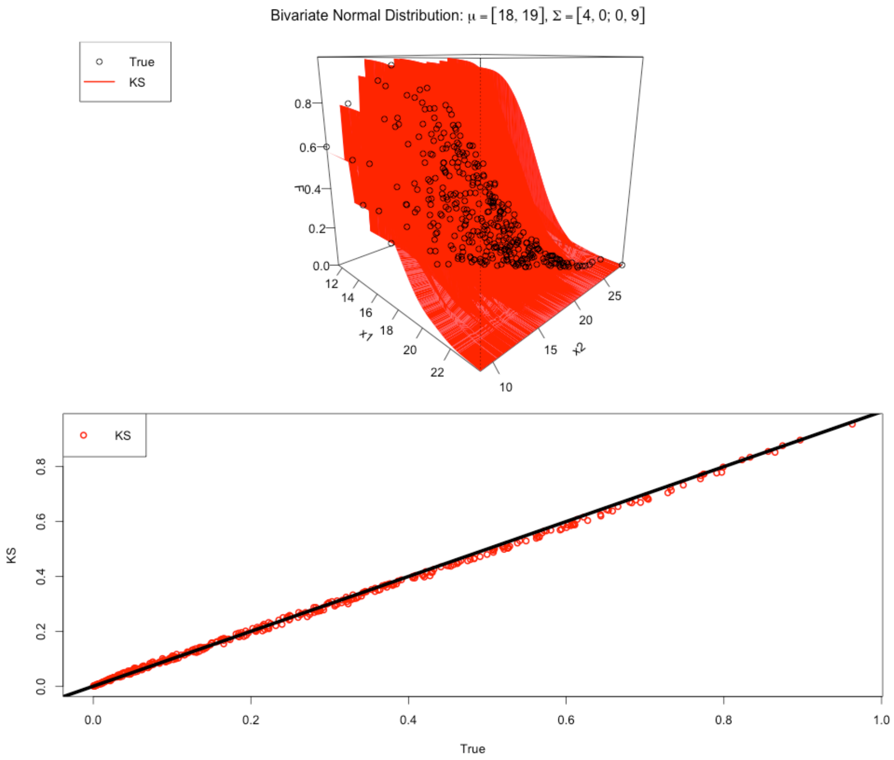
- Artificially generated historical data
  - Normal distributions with μ = [18; 19] and Σ = [4, 0; 0, 9].
- Compared KDE-based reformulation solutions with Exact reformulation
- Modeled in AIMMS 3.13.5 with GUROBI 5.1 (LP) and IPOPT 3.10.1 (NLP).

Artificial Historical Data

Data and Quantile Estimation for (PPICC)

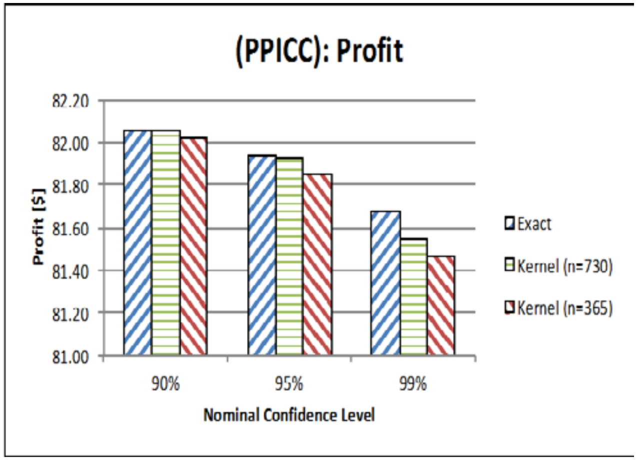


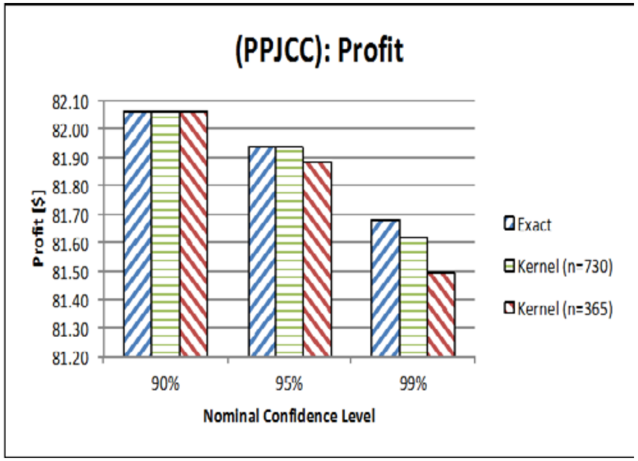
Data and Joint CDF Estimation for (PPJCC)



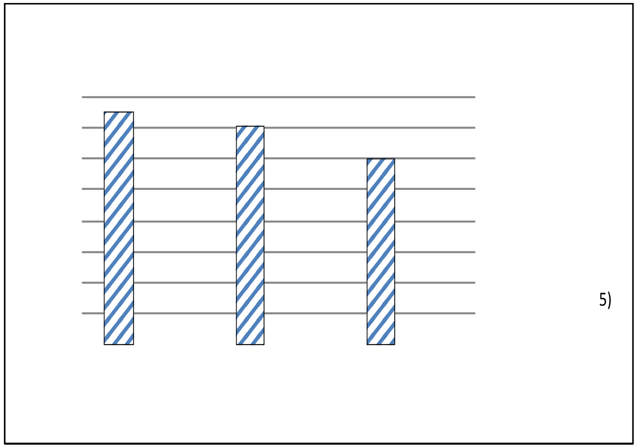
Results

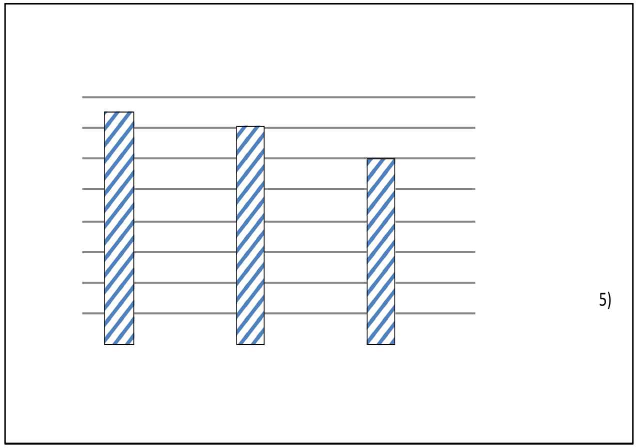
- Profits





- Flowrates out of *P3*





Conclusions

- Kernel smoothing: data-driven statistical method for reformulating chance constraints with RHS uncertainty.
- Use of density-based confidence set with ϕ-divergence. Specification of the divergence tolerance *d* from distribution of squared point-wise standard errors estimated from the KDE process.
- Sample size influences the accuracy of the estimation, and ultimately, the quality of solution.
- ICC problem is generally easier to solve. Can use its solution to initialize the JCC problem.

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