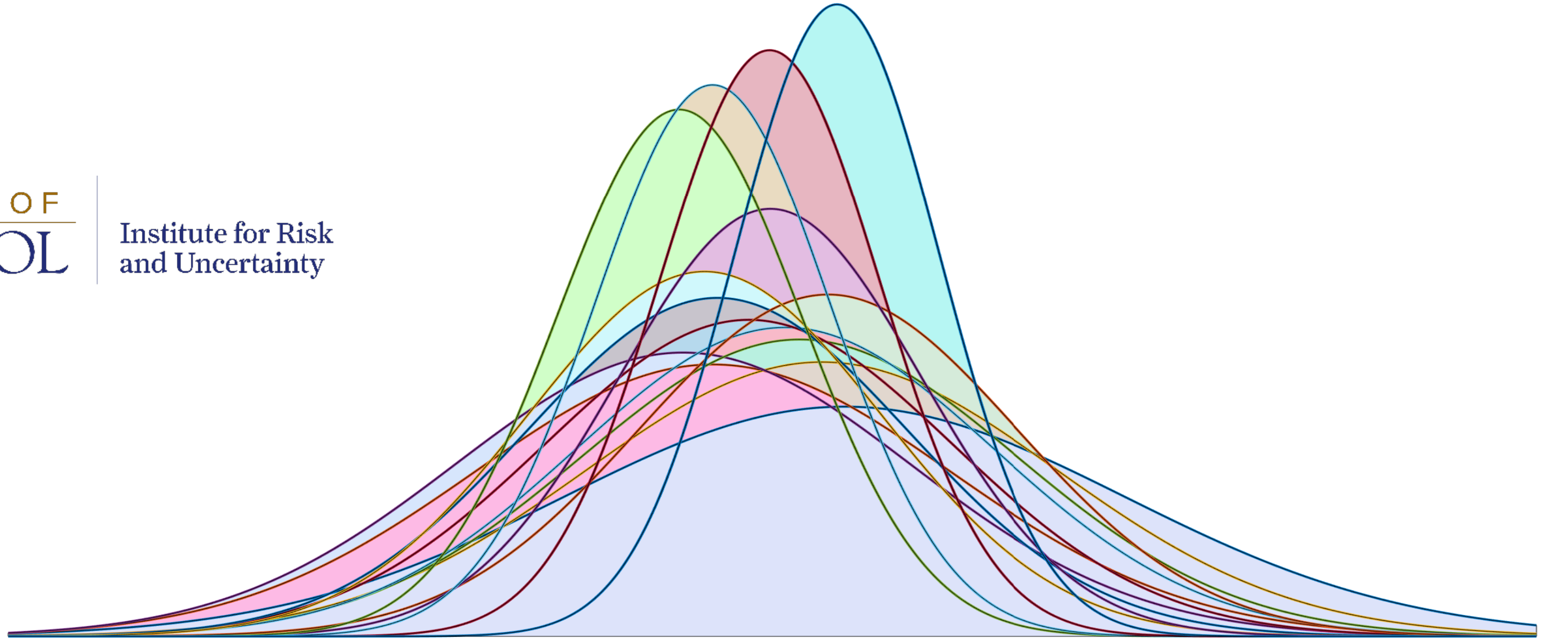
Distribution-free uncertainty propagation



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Monte Carlo

- Most popular uncertainty propagation
- Non-intrusive

- Requires specified distributions
- Requires dependence assumptions
- Doesn’t consider its own reliability
- Can’t see individual variance components

First order error propagation

- In probability theory called “*Moment propagation*”
- Propagates mean & variance through mathematical expressions
- Although widely used, requires a lot of assumptions, and does not inform about distribution shape

Pessimism from Cullen and Frey (1999)

- Bad for risk analysis:
  - Requires stochastic independence
  - Moments must be perfectly known
  - Gives no information about tails without distribution assumption
  - Only accurate for near-linear models

Moment Arithmetic

- Generalisation with the following:
  - Independence between variables need not be assumed
  - Moment propagation formulae may be evaluated with intervals
  - Assumptions about input distributions is no longer necessary
  - Works for non-linear functions

Moment Arithmetic

- Computer arithmetic on random variable's *range, mean* and *variance*
- 7 binary operations: +, -, *, /, ^, min, max
- 9 unary operations: rescale, shift, exp, log, ln, 1/*x*, x^2, $\sqrt{x}$, $|x|$
- For independence and unknown dependence (Fréchet)

https://github.com/AnderGray/MomentArithmetic.jl

Interval arithmetic

	Least possible value	*Greatest possible value*
$k + X$ (shifting)	$\mathbf{k} + \underline{\mathbf{X}}$	$\mathbf{k} + \overline{\mathbf{X}}$
kX (rescaling)	$\begin{cases} \mathbf{k}\underline{\mathbf{X}}, & \text{if } 0 \leq k \\ \mathbf{k}\overline{\mathbf{X}}, & \text{if } k < 0 \end{cases}$	$\begin{cases} \mathbf{k}\overline{\mathbf{X}}, & \text{if } 0 \leq k \\ \mathbf{k}\underline{\mathbf{X}}, & \text{if } k < 0 \end{cases}$
e^X	$\mathbf{e}^{\underline{\mathbf{X}}}$	$\mathbf{e}^{\overline{\mathbf{X}}}$
$\ln(X)$ for $0 < X$	$\mathbf{ln}(\underline{\mathbf{X}})$	$\mathbf{ln}(\overline{\mathbf{X}})$
$\log_{10}(X)$ for $0 < X$	$\mathbf{log_{10}}(\underline{\mathbf{X}})$	$\mathbf{log_{10}}(\overline{\mathbf{X}})$
$\frac{1}{X}$ for $0 \notin X$	$\mathbf{1}/\overline{\mathbf{X}}$	$\mathbf{1}/\underline{\mathbf{X}}$
X^2	$\begin{cases} \mathbf{0}, & \text{if } 0 \in X \\ \mathbf{min}(\underline{\mathbf{X}}^{\mathbf{2}}, \overline{\mathbf{X}}^{\mathbf{2}}), & \text{otherwise} \end{cases}$	$\mathbf{max}(\underline{\mathbf{X}}^{\mathbf{2}}, \overline{\mathbf{X}}^{\mathbf{2}})$
$\lvert X \rvert$ (absolute value)	$\begin{cases} \mathbf{0}, & \text{if } 0 \in X \\ \mathbf{min}(\lvert\underline{\mathbf{X}}\rvert, \lvert\overline{\mathbf{X}}\rvert), & \text{otherwise} \end{cases}$	$\mathbf{max}(\lvert\underline{\mathbf{X}}\rvert, \lvert\overline{\mathbf{X}}\rvert)$
$\sqrt{X}$ for $0 \leq X$	$\sqrt{\underline{\mathbf{X}}}$	$\sqrt{\overline{\mathbf{X}}}$
$X + Y$	$\underline{\mathbf{X}} + \underline{\mathbf{Y}}$	$\overline{\mathbf{X}} + \overline{\mathbf{Y}}$
$X - Y$	$\underline{\mathbf{X}} - \overline{\mathbf{Y}}$	$\overline{\mathbf{X}} - \underline{\mathbf{Y}}$
$X \times Y$	$\mathbf{min}(\underline{\mathbf{X}}\underline{\mathbf{Y}}, \underline{\mathbf{X}}\overline{\mathbf{Y}}, \overline{\mathbf{X}}\underline{\mathbf{Y}}, \overline{\mathbf{X}}\overline{\mathbf{Y}})$	$\mathbf{max}(\underline{\mathbf{X}}\underline{\mathbf{Y}}, \underline{\mathbf{X}}\overline{\mathbf{Y}}, \overline{\mathbf{X}}\underline{\mathbf{Y}}, \overline{\mathbf{X}}\overline{\mathbf{Y}})$
$\frac{X}{Y}$ for $0 \notin Y$	$\mathbf{min}(\underline{\mathbf{X}}/\underline{\mathbf{Y}}, \underline{\mathbf{X}}/\overline{\mathbf{Y}}, \overline{\mathbf{X}}/\underline{\mathbf{Y}}, \overline{\mathbf{X}}/\overline{\mathbf{Y}})$	$\mathbf{max}(\underline{\mathbf{X}}/\underline{\mathbf{Y}}, \underline{\mathbf{X}}/\overline{\mathbf{Y}}, \overline{\mathbf{X}}/\underline{\mathbf{Y}}, \overline{\mathbf{X}}/\overline{\mathbf{Y}})$
X^Y for $0 < X$ or $0 < Y$	$\mathbf{min}(\underline{\mathbf{X}}^{\underline{\mathbf{Y}}}, \underline{\mathbf{X}}^{\overline{\mathbf{Y}}}, \overline{\mathbf{X}}^{\underline{\mathbf{Y}}}, \overline{\mathbf{X}}^{\overline{\mathbf{Y}}})$	$\mathbf{max}(\underline{\mathbf{X}}^{\underline{\mathbf{Y}}}, \underline{\mathbf{X}}^{\overline{\mathbf{Y}}}, \overline{\mathbf{X}}^{\underline{\mathbf{Y}}}, \overline{\mathbf{X}}^{\overline{\mathbf{Y}}})$
$\min(X, Y)$	$\mathbf{min}(\underline{\mathbf{X}}, \underline{\mathbf{Y}})$	$\mathbf{min}(\overline{\mathbf{X}}, \overline{\mathbf{Y}})$
$\max(X, Y)$	$\mathbf{max}(\underline{\mathbf{X}}, \underline{\mathbf{Y}})$	$\mathbf{max}(\overline{\mathbf{X}}, \overline{\mathbf{Y}})$

Arithmetic with independence

	Mean	*Variance*
$X+Y$	$\mathbf{EX}+\mathbf{EY}$	$\mathbf{VX}+\mathbf{VY}$
$X-Y$	$\mathbf{EX}-\mathbf{EY}$	$\mathbf{VX}+\mathbf{VY}$
$X\times Y$	$\mathbf{EXEY}$	$(\mathbf{EX})^2\mathbf{VY}+(\mathbf{EY})^2\mathbf{VX}+\mathbf{VXVY}$
$\frac{X}{Y}$ for $0\notin Y$	$E(X\times(1/Y))$	$V(X\times(1/Y))$
X^Y for $0<X$ or $0<Y$	$E(\exp(\ln(X)\times Y))$	$V(\exp(\ln(X)\times Y))$
$\max(X,Y)$	$\begin{cases}\mathbf{EX}, & \text{if } Y<X\\ \mathbf{EY}, & \text{if } X<Y\\ \text{“Bertsimas max”}, & \text{otherwise}\end{cases}$	$\begin{cases}\mathbf{VX}, & \text{if } Y<X\\ \mathbf{VY}, & \text{if } X<Y\\ \text{env}(\max(VX,VY),0), & \text{otherwise}\end{cases}$
$\min(X,Y)$	$\begin{cases}\mathbf{EX}, & \text{if } X<Y\\ \mathbf{EY}, & \text{if } Y<X\\ \text{“Bertsimas min”}, & \text{otherwise}\end{cases}$	$\begin{cases}\mathbf{VX}, & \text{if } X<Y\\ \mathbf{VY}, & \text{if } Y<X\\ \text{env}(\max(VX,VY),0), & \text{otherwise}\end{cases}$

Yields intervals

Arithmetic without dependence assumptions (Fréchet)

	Mean	*Variance*
$k + X$ (shifting)	$\mathbf{k + EX}$	$\mathbf{VX}$
kX (rescaling)	$\mathbf{kEX}$	$\mathbf{k^2VX}$
e^X	rowe(exp)	rowevar(exp)
$\ln(X)$ for $0 < X$	rowe(ln)	rowevar(ln)
$\log_{10}(X)$ for $0 < X$	rowe($\log_{10}$)	rowevar($\log_{10}$)
$\frac{1}{X}$ for $0 \notin X$	rowe(reciprocal)	rowevar(reciprocal)
X^2	$\mathbf{(EX)^2 + VX}$	rowevar(square)
$\lvert X \rvert$ (absolute value)	$\begin{cases} \mathbf{EX}, & \text{if } 0 \leq \underline{X} \\ -\mathbf{EX}, & \text{if } \overline{X} \leq 0 \\ [\lvert EX \rvert, \lvert EX \rvert + \sqrt{VX}(\pi - \text{atan}(\frac{\lvert EX \rvert}{\sqrt{VX}}))], & \text{if } 0 \in X \end{cases}$	$\max(0, EX^2 + VX - E(\lvert X \rvert)^2)$
$\sqrt{X}$ for $0 \leq X$	rowe($\surd$)	rowevar($\surd$)
$X + Y$	$\mathbf{EX + EY}$	$\mathbf{(\sqrt{VX} \pm \sqrt{VX})^2}$
$X - Y$	$\mathbf{EX - EY}$	$\mathbf{(\sqrt{VX} \pm \sqrt{VX})^2}$
$X \times Y$	$\mathbf{EXEY \pm \sqrt{VXVY}}$	"Goodman"
$\frac{X}{Y}$ for $0 \notin Y$	$E(X \times (1/Y))$	$V(X \times (1/Y))$
X^Y for $0 < X$ or $0 < Y$	$E(\exp(\ln(X) \times Y))$	$V(\exp(\ln(X) \times Y))$
$\max(X, Y)$	"Bertsimas max"	$\text{env}(\max(VX, VY), 0)$
$\min(X, Y)$	"Bertsimas min"	$\text{env}(\max(VX, VY), 0)$

Scattered across the literature

- Formula for variance (Goodman)
- Transformations with constant-sign derivatives (Rowe)
- Formulas can often be tighter (Kreinovich)
- Max and min functions (Bertsimas)
- Homegrown inequalities

Rowe formulas for moment transformations

- Formulas for constant-sign-derivative transformations
- $t = \{\exp, \ln, \log, 1/x, \sqrt{x}\}$

$$\mathrm{rowe}(t) = \mathrm{env}(Pt(\underline{X}) + (1-P)t(EX + \frac{VX}{EX - \underline{X}}), Qt(\overline{X}) + (1-Q)t(EX + \frac{VX}{EX - \overline{X}})) \quad (1)$$

$$\mathrm{rowevar}(t) = \mathrm{env}(\frac{t(\underline{\nu}) - t(\underline{X})}{(\underline{\nu} - \underline{X})^2}(VX + (\underline{\nu} - EX)^2), \frac{t(\overline{\nu}) - t(\overline{X})}{(\overline{\nu} - \overline{X})^2}(VX + (\overline{\nu} - EX)^2)) \quad (2)$$

$$P = 1/(1 + (EX - \underline{X})^2/VX)$$

$$Q = 1/(1 + (EX - \overline{X})^2/VX)$$

Rowe, N. C., Absolute bounds on the mean and standard deviation of transformed data for constant-sign-derivative transformations, SIAM journal on scientific and statistical computing 9 (6) (1988) 1098–1113.

Goodman variance for product

$$V(XY) = (EX)^2 VY + (EY)^2 VX + 2EXEYE_{11} + 2EXE_{12} + 2EYE_{21} + E_{22} - E_{11}^2$$

$$E_{ij} = E[(X - EX)^i (Y - EY)^j] \text{ (e.g. } E_{11} \text{ is covariance)}$$

$$\begin{aligned} E_{11} &= E[(X - EX)(Y - EY)] \\ &= E[XY - XEY - YEX + EXEY] \\ &= E[XY] - EXEY \end{aligned}$$

Goodman, L. A., On the exact variance of products, Journal of the American statistical association 55 (292) (1960) 708–713.

Goodman variance for product

$$
\begin{aligned}
E_{21} &= E[(X - EX)^2(Y - EY)] \\
&= E[X^2Y + E[X]^2Y - X^2E[Y] + 2E[X]E[Y]X - 2E[X]XY - E[X]^2E[Y]] \\
&= E[X^2Y] + E[X]^2E[Y] - E[X^2]E[Y] + 2E[X]^2E[Y] - 2E[X]E[XY] - E[X]^2E[Y] \\
&= E[X^2Y] - E[X^2]E[Y] + 2E[X]^2E[Y] - 2E[X]E[XY]
\end{aligned}
$$

$$
\begin{aligned}
E_{22} &= E[(X - EX)^2(Y - EY)^2] \\
&= E[E[X]^2E[Y]^2 - 2E[X]E[Y]^2X + E[Y]^2X^2 - 2E[X]^2E[Y]Y + 4E[X]E[Y]XY \\
&\quad -2E[Y]X^2Y + E[X]^2Y^2 - 2E[X]XY^2 + X^2Y^2] \\
&= E[X]^2E[Y]^2 - 2E[X]^2E[Y]^2 + E[Y]^2E[X^2] - 2E[X]^2E[Y]^2 + 4E[X]E[Y]E[XY] \\
&\quad -2E[Y]E[X^2Y] + E[X]^2E[Y^2] - 2E[X]E[XY^2] + E[X^2Y^2] \\
&= -3E[X]^2E[Y]^2 + E[X^2]E[Y]^2 + E[X]^2E[Y^2] + 4E[X]E[Y]E[XY] \\
&\quad -2E[Y]E[X^2Y] - 2E[X]E[XY^2] + E[X^2Y^2]
\end{aligned}
$$

Using the tables with intervals

- Tables can be readily evaluated with *interval arithmetic*
- *EX, VX,* and bounds can be intervals
- Repeated variables
- Subintervalisation: n^m interval calculations
- Since only 2 variables are intervals, subintervalisation works well
- $n \approx 20\,; m = 2$

Missing information

Mean and variance bounds can be estimated from range

```
julia> A = Moments(mean = missing, var = missing, range = interval(2.3, 7))
moment:              ~ ( mean = [2.3,7.0], var = [0.0,5.5225] , range = [2.3,7.0] )

julia> B = Moments(mean = 3, var = missing, range = interval(2.3, 7))
moment:              ~ ( mean  = 3, var = [0.0,2.8000000000000007] , range = [2.3,7.0] )

julia> C = Moments(mean = interval(5, 10), var = missing, range = interval(2.3, 7))
moment:              ~ ( mean = [5.0,7.0], var = [0.0,5.4] , range = [2.3,7.0] )

julia> D = Moments(mean = interval(10, 30), var = missing, range = interval(2.3, 7))
ERROR: ArgumentError: Provided information not valid. Mean ∩ Range = ∅.
       [10, 30] ∩ [2.29999, 7] = ∅
julia> E = Moments(mean = 3, var = interval(15,18), range = interval(2.3, 7))
ERROR: ArgumentError: Provided information not valid. Variance ∩ VarBounds = ∅.
       [15, 18] ∩ [0, 2.80001] = ∅
```

Mean and variance bounded from ranges

Tighter variance when mean is given

Given mean is too wide

Inconsistent mean

Inconsistent variance

Example: mink dietary mercury

$$TDI = FMR \,|\times|\, \left(\frac{C_{\text{fish}} \,|\times|\, P_{\text{fish}}}{AE_{\text{fish}} \,|\times|\, GE_{\text{fish}}} + \frac{C_{\text{inverts}} \,|\times|\, P_{\text{inverts}}}{AE_{\text{inverts}} \,|\times|\, GE_{\text{inverts}}} \right)$$

C_{fish}, C_{inverts}	mercury concentration in fish or invertebrate tissue
P_{fish}, P_{inverts}	proportion of fish or inverts in the mammal's diet
GE_{fish}, GE_{inverts}	gross energy of fish or invertebrate tissue
AE_{fish}, AE_{inverts}	assimilation efficiency for dietary fish or inverts
FMR	normalized free metabolic rate
BW	body mass of the mammal

Hibernian Mink

Input ranges and moments

	Min	Max	Mean	Stdev	Units
GE_{fish}	500	2000	1200	240	Kcal per kg
$GE_{inverts}$	300	1700	1050	225	Kcal per kg
AE_{fish}	0.77	0.98	0.91	?	
$AE_{inverts}$	0.72	0.96	0.87	?	
C_{fish}	0.1	0.3	?	?	mg per kg
$C_{inverts}$	0.02	0.06	?	?	mg per kg
P_{fish}	0.9	0.9	0.9	0	
$P_{inverts}$	0.1	1.0	0.9	0	
BW	400	800	608	66.9	gram

$\text{TDI} = \text{FMR} \;|*|\; (C_{fish} * P_{fish} / (AE_{fish} |*| GE_{fish}) + C_{inverts} * P_{inverts} / (AE_{inverts} |*| GE_{inverts})$

$\text{FMR} = [0.412 \pm 0.058] * \text{mag}(BW) \wedge [0.862 \pm 0.026] * 1$ Kcal per kg per day

(vertical bars denote independence between the operands)

Total daily intake, mg per kg per day

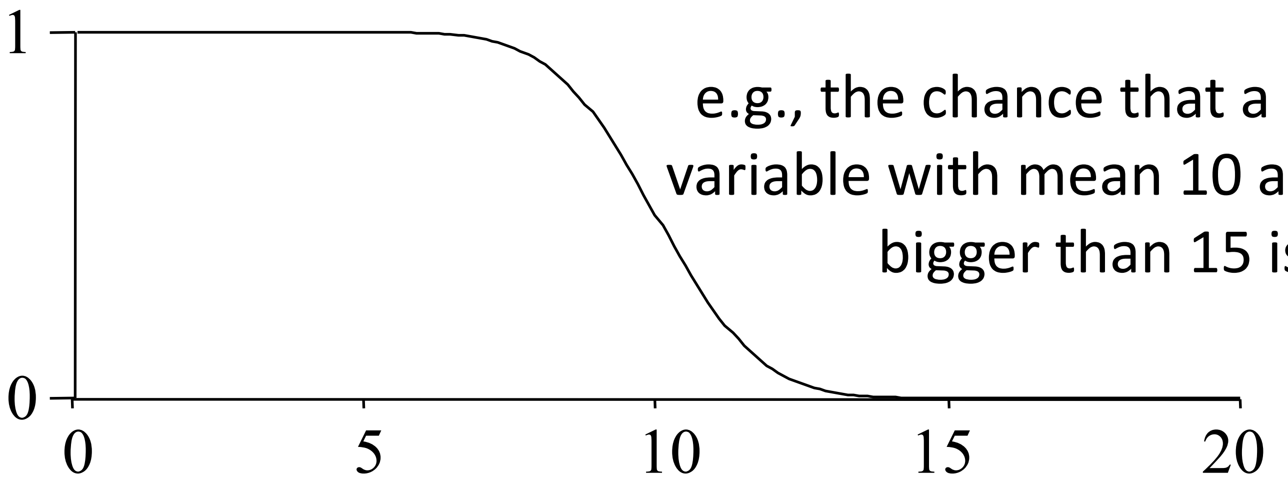
Mean	[0.06,0.47]
Stdev	[0.04, 0.51]
Max	1.19

Useful information even though some inputs were totally unknown

What do range and moments say about risks?

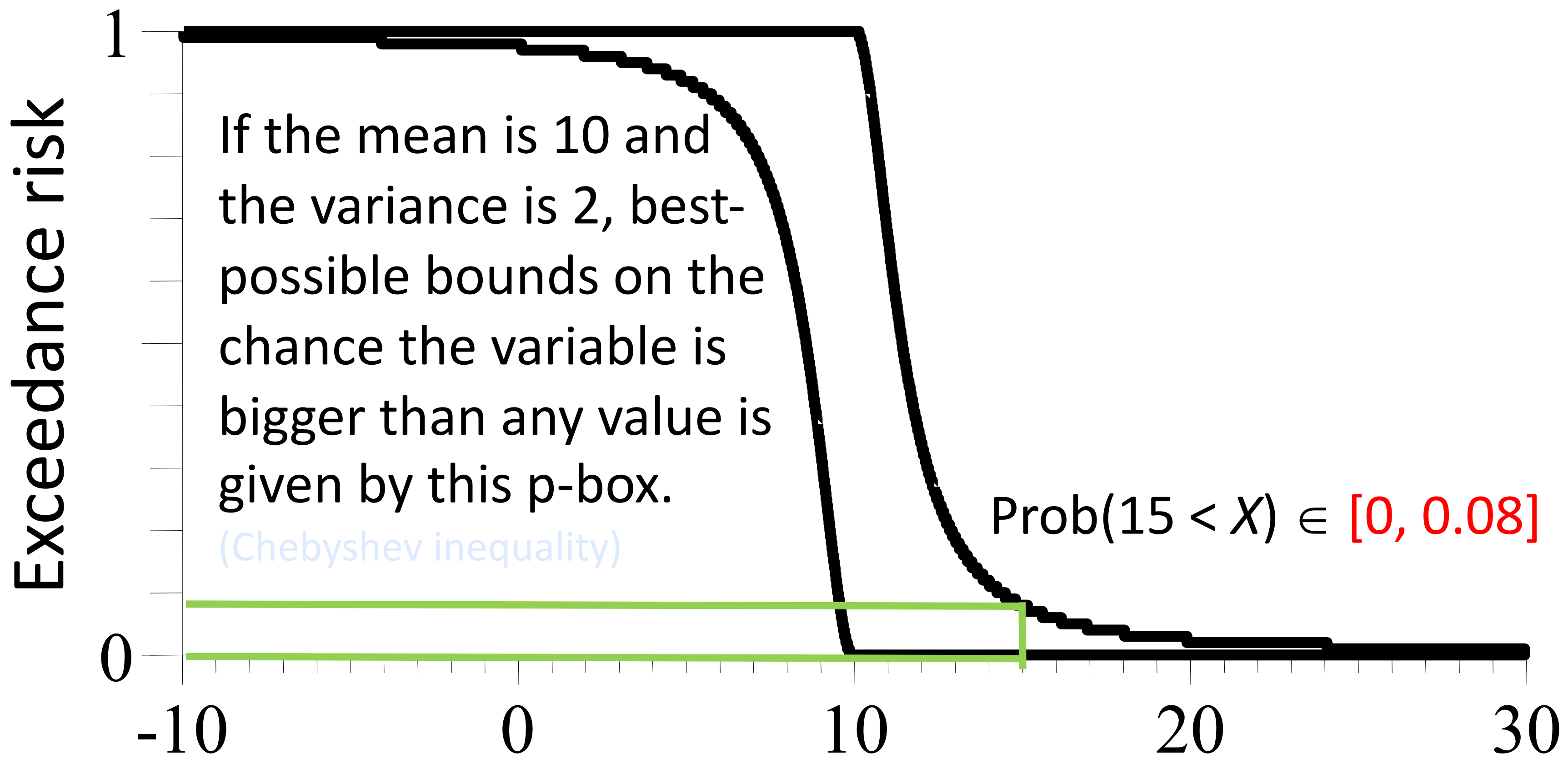
Traditional normal theory

- Distribution determined by mean and variance
- Probability in tails drops quickly



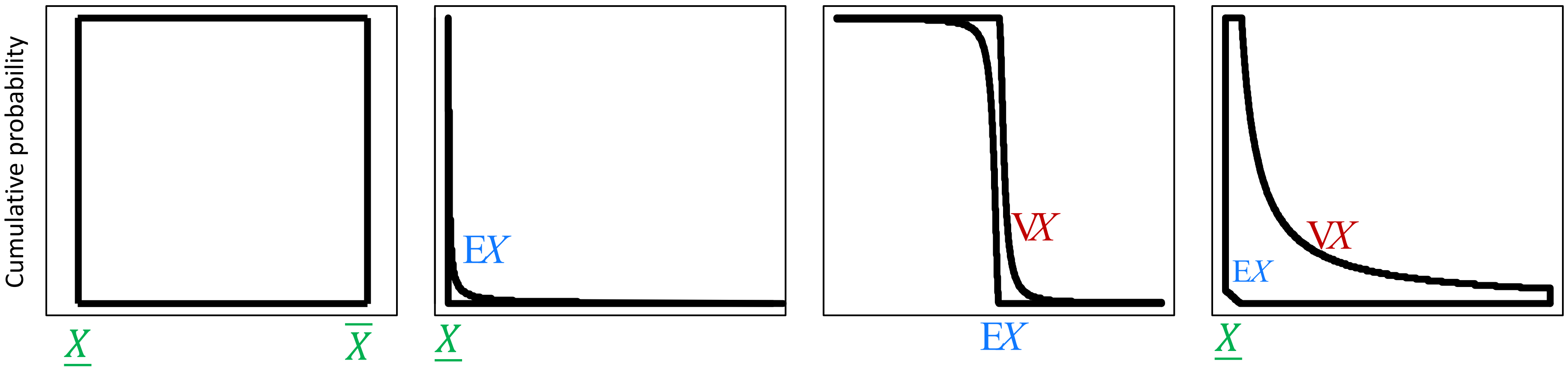
e.g., the chance that a normal random variable with mean 10 and variance 2 is bigger than 15 is only 0.000203

What do moments say about risks?

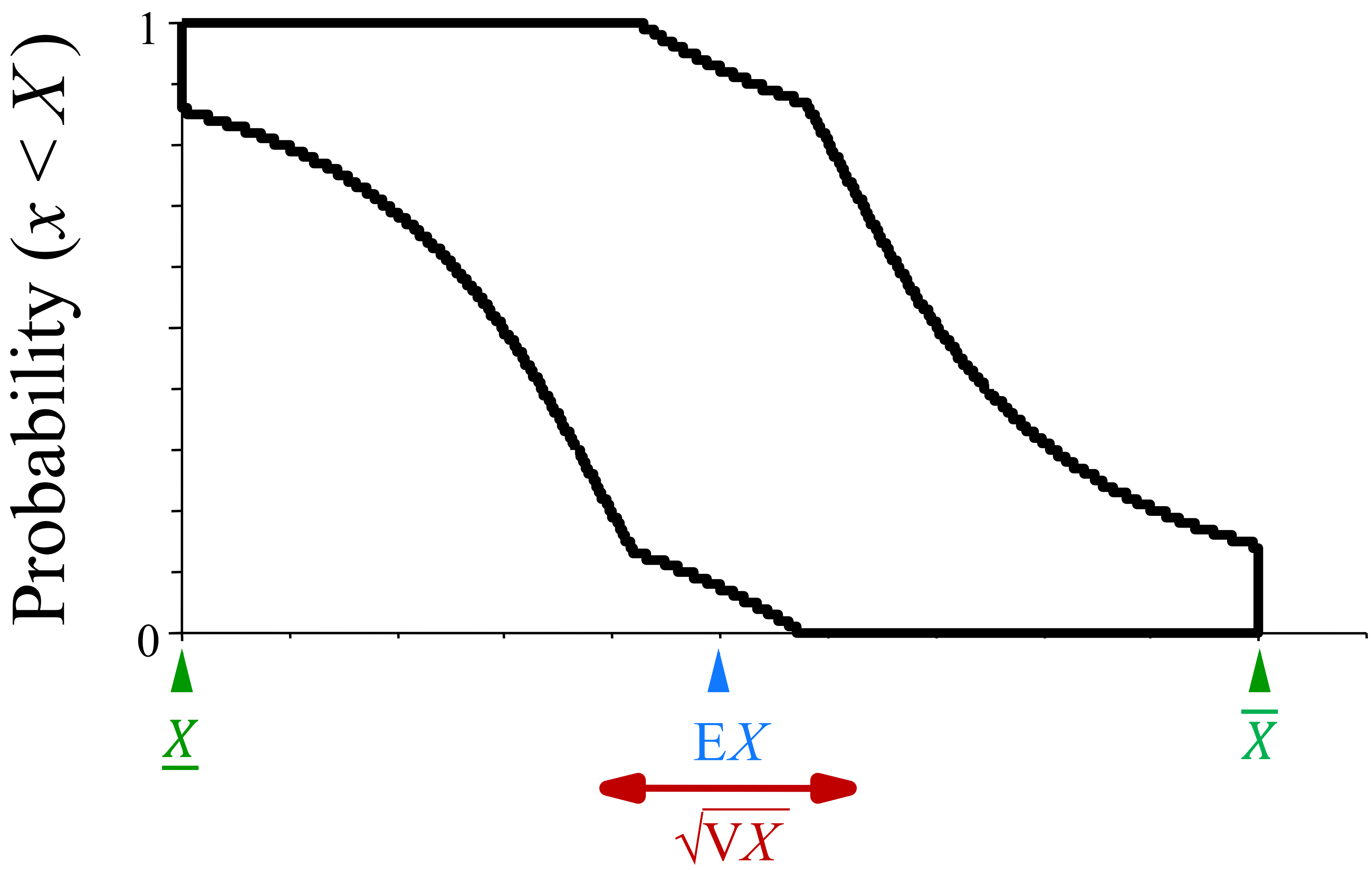


Constraining probabilities and quantiles

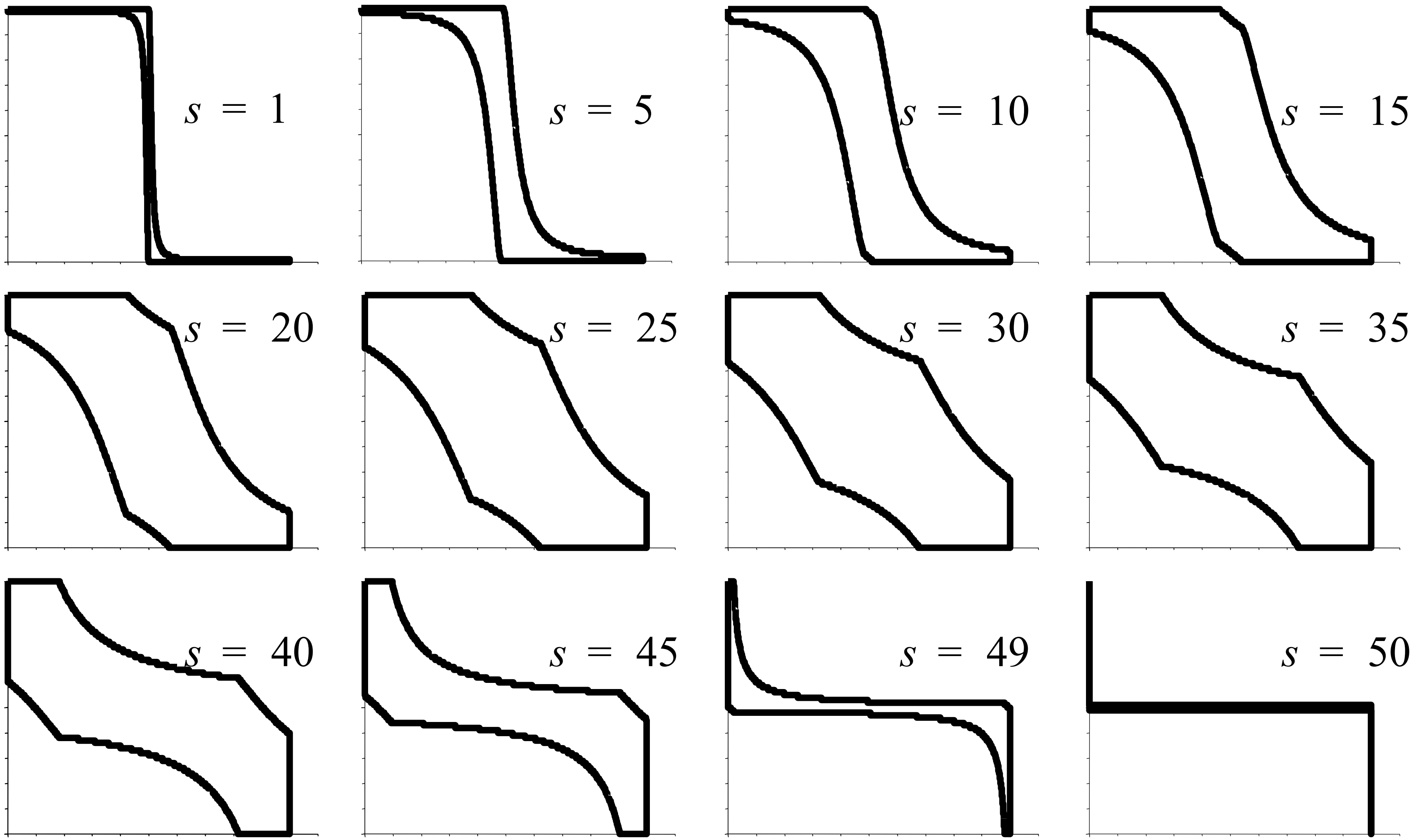
- Interval $\{\underline{X}, \overline{X}\}$
- Markov $\{\underline{X}, EX\}, \{EX, \overline{X}\}$
- Chebyschev $\{EX, VX\}$
- Cantelli $\{\underline{X}, EX, \text{VX}\}, \{EX, VX, \overline{X}\}$



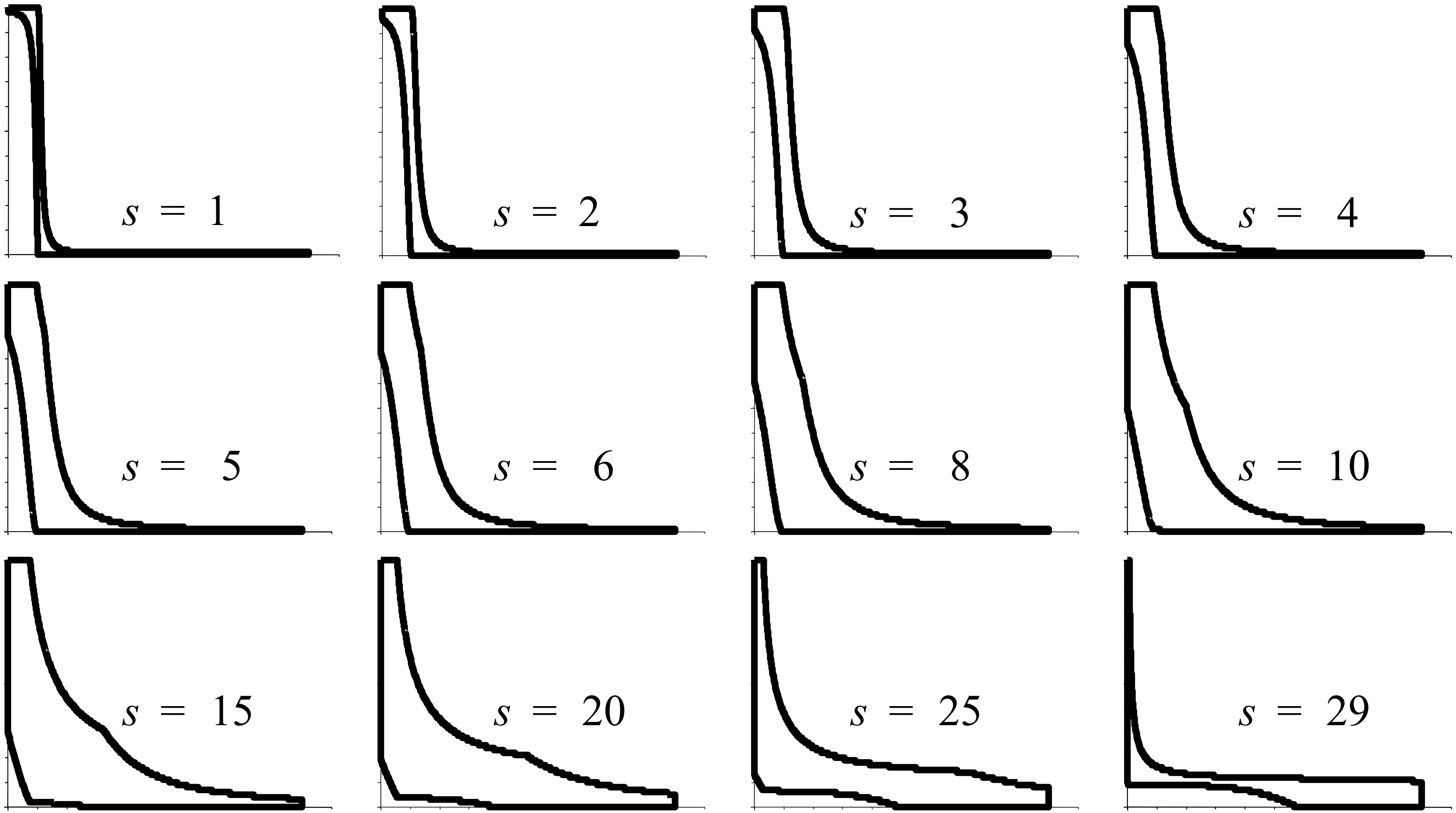
Range and moments *together*



{min = 0, max = 100, mean = 50, stdev = s}



{min = 0, max = 100, mean = 10, stdev = s}



Moment arithmetic: *distribution-free* risk analysis

- Fully probabilistic (with tails)
- Rigorous rather than approximate
- Needs no distributions, dependencies, derivatives
- Some moments/bounds can be totally unknown

- Bounds may be too wide to be useful
- Requires dependency tracking
- Intrusive

Grazie

Covariance arithmetic

$$Z = X + Y \qquad VZ = VX + 2\mathrm{Cov}[X, Y] + VY$$

$$Z = X - Y \qquad VZ = VX - 2\mathrm{Cov}[X, Y] + VY$$

$$Z = X * Y \qquad VZ = \text{Goodman}$$

$$Z = X / Y \qquad VZ = V[X * (1/Y)]$$

Springer, Melvin Dali. *The algebra of random variables*. No. 519.2 S67. 1979

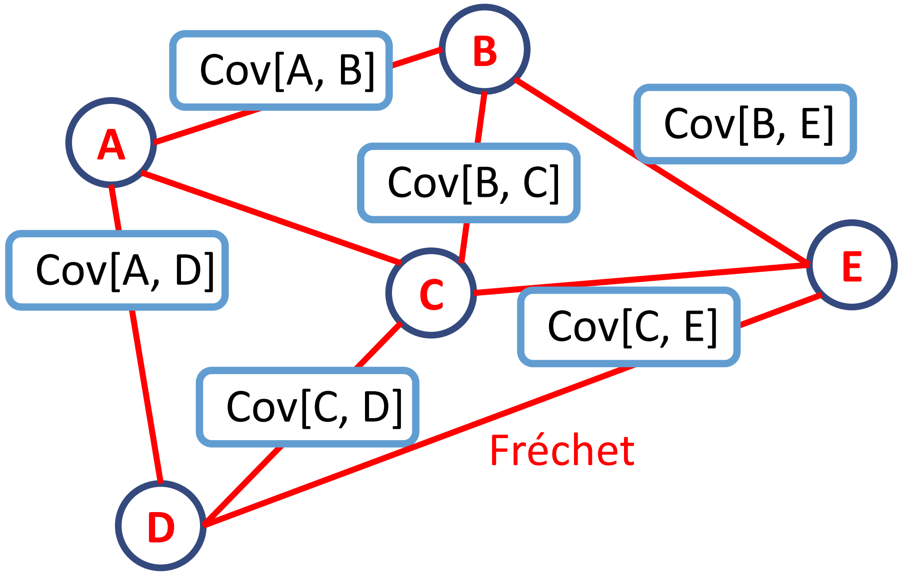
Covariance tracking

	$Z = X + Y$	$\text{Cov}[Z, X] = VX + \text{Cov}[X, Y]$
	$Z = X - Y$	$\text{Cov}[Z, X] = VX - \text{Cov}[X, Y]$
	$Z = X * Y$	$\text{Cov}[Z, X] = E[X^2 Y] - E[XY]EX$
(Numerator)	$Z = X / Y$	$\text{Cov}[Z, X] = E[X^2/Y] - E[X/Y]EX$
(Denominator)	$Z = X / Y$	$\text{Cov}[Z, Y] = EX - E[X/Y]EY$

Springer, Melvin Dali. *The algebra of random variables*. No. 519.2 S67. 1979

Covariance tracking

- Graphical model for storing dependencies
- Nodes are moment variables
- Edges are covariances
- Make a new node and edge when a variable is created



Cov[B, C]

$$E = B + C$$

Cov[C, E] Cov[B, E]

$$F = D + E$$

Fréchet

Covariance tracking

The graph is an ill-specified covariance matrix

$$\begin{array}{c|cccc} & A & B & C & D \\ \hline A & VA^2 & C[A,B] & C[A,C] & C[A,D] \\ B & C[B,A] & VB^2 & C[B,C] & ??? \\ C & C[C,A] & C[C,B] & VC^2 & ??? \\ D & C[D,A] & ??? & ??? & VD^2 \end{array}$$

$D = A + C$