Instructions

1. Read the slide notes (under each slide)
2. Review the slide for the main messages
3. Answer questions (correct answers at end)
4. Some advanced/optional slides also at end
   - After completing a slide…

SC.63 - SC.65

…means <u>optionally</u> proceed to SC.63-SC.65

5. If unsure: james.brown@hydrosolved.com

1st HEFS workshop, 08/19/2014

Basic Hydrologic Ensemble Theory (for review in Seminar C)

James Brown

james.brown@hydrosolved.com

Contents

1. Why use ensemble forecasting?
2. What are the sources of uncertainty?
3. How to quantify the input uncertainties?
4. The ingredients of a probability model
5. How to quantify the output uncertainties?
6. How to apply operationally?

What is not covered?

Limited scope

- Not a mathematical/statistical primer
- Not a literature review of current techniques
- Focus on the basic theory of ensemble forecasting
- Does not cover theory of hindcasting and verification

Limited detail

- Mathematical detail often sacrificed
- Not focused on HEFS techniques (addressed later)
- For more details, see linked resources (end of slides)

1. Why use ensemble forecasting?

Reasons to assess uncertainty

Single-valued forecasts are misleading

- There is an understandable desire for simplicity
- Yet, also known that large uncertainties are common
- Ignoring them can lead to wrong/impaired decisions
- Uncertainties “propagate” (e.g. met > hydro > eco)

Risk-based decision making

- Knowledge of uncertainty helps to manage risks
- E.g. risk of false warnings tied to flood probability
- E.g. risk of excess releases tied to inflow probability

National Research Council, 2006

"All prediction is inherently uncertain and effective communication of uncertainty information in weather, seasonal climate, and hydrological forecasts benefits users' decisions (e.g. AMS, 2002; NRC; 2003b). The chaotic character of the atmosphere, coupled with inevitable inadequacies in observations and computer models, results in forecasts that always contain uncertainties. These uncertainties generally increase with forecast lead time and vary with weather situation and location. *Uncertainty is thus a fundamental characteristic of weather, seasonal climate, and hydrological prediction, and no forecast is complete without a description of its uncertainty.*" [emphasis added]

COMPLETING THE FORECAST

Characterizing and communicating Uncertainty for Better Decisions Using Weather and Climate Forecasts

Committee on Estimating and Communicating Uncertainty in Weather and Climate Forecasts

Board on Atmospheric Sciences and Climate

Division on Earth and Life Studies

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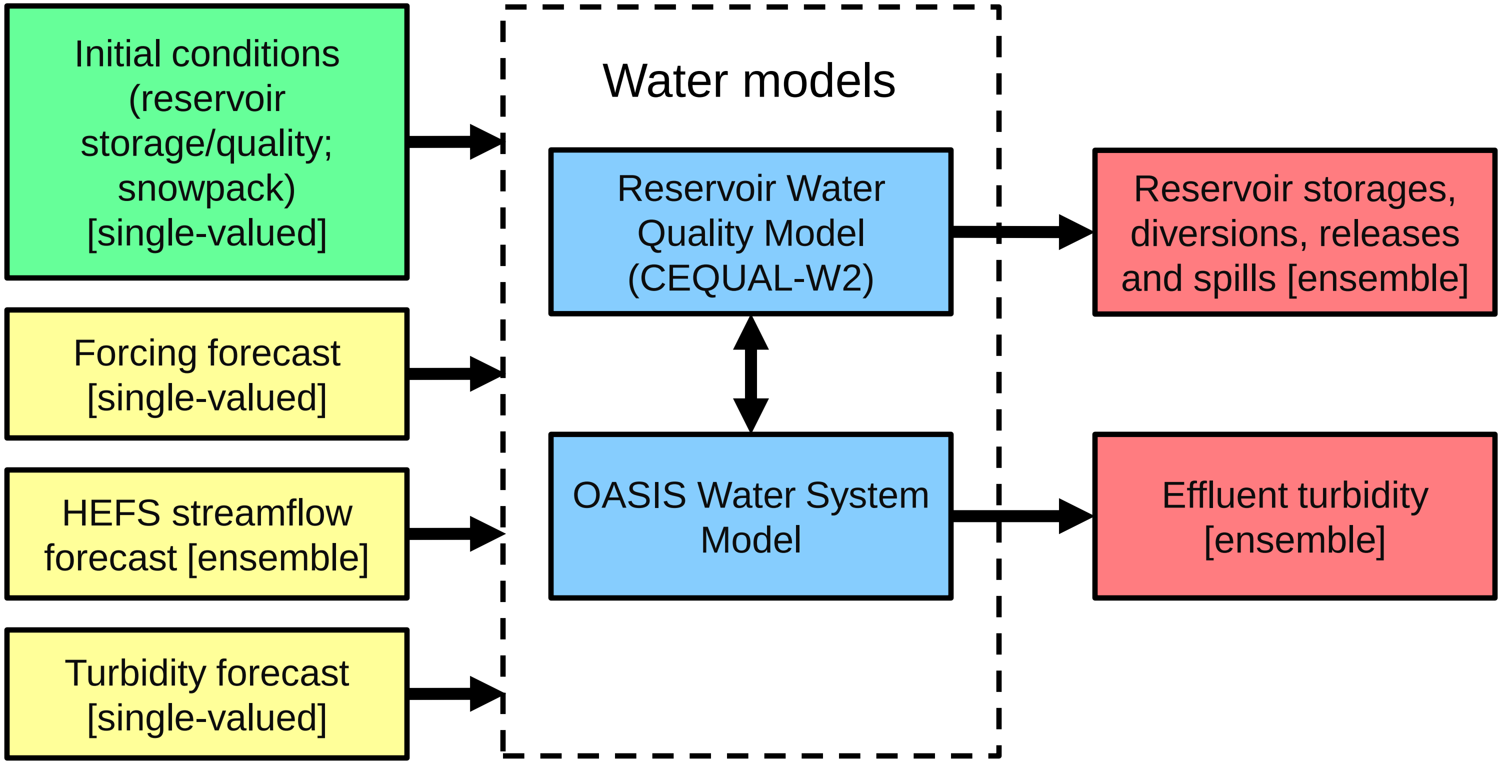
Example application

- HEFS inputs to NYCDEP Operational Support Tool (OST)



- Output: risks to volume objectives (e.g. habitat, flooding)
- Output: risks to quality objectives (NYC water supply)

Reasons to not assess uncertainty

In the interests of balance…

- Technical details risk knowledge/communication gap
- Scope for misunderstanding probabilities…
- …for example, may not consider all uncertainties
- Large upfront investment (in systems and training)

But justified for operational forecasting

- For operations, balance strongly favors ensembles
- Reflected in investments (NWS, ECMWF, BoM..)
- BUT: training and communication is a long-term effort

Reasons to use ensemble technique

Ensemble Prediction Systems

- Highly practical tool to “propagate” uncertainty
- Based on running models with multiple scenarios
- Scenario is one combination of model settings
- Need to include all main settings/uncertainty sources

Advantages

- Flexible: just run existing (chain of) models n times
- Scalable: allows complex models, parallel processing
- Collaborative: widely used in meteorology etc.

History of ensembles in NWS

Focused on long-range

- Ensemble Streamflow Prediction (since late 1970s)
- Climate ensemble from past weather observations
- Various adaptations (e.g. to use CPC outlooks)

Limitations of ESP

- Not based on forecasts, so only reproduces the past
- Does not use best data for short-/medium-range
- Does not account for hydrologic uncertainties/biases
- Hydrologic uncertainties/biases can exceed meteo.!

Need for an end-to-end system

HEFS service objectives

- HEFS “A Team” defined several requirements:

1. Span lead times from hours to years, seamlessly
2. Issue reliable probabilities (capture total uncertainty)
3. Be consistent in space/time, linkable across domains
4. Use available meteorological forecasts, correct biases
5. Provide hindcasts consistent w/ operational forecasts
6. Support verification of the end-to-end system

- These requirements are built into HEFS theory

Question 1: check all that apply

What are the limitations of NWS-ESP?

- ☐ A. Does not model forcing uncertainty
- ☐ B. Does not model hydrologic uncertainty
- ☐ C. Does not model total uncertainty
- ☐ D. Does not use short/medium-range forecast forcing
- ☐ E. Is not based on calibrated hydrologic models
- ☐ F. Does not correct for biases

- Answers are at the end.

2. What are the main sources of uncertainty?

Main sources of uncertainty

Total uncertainty in hydrologic forecasts

- Originates from two main sources:

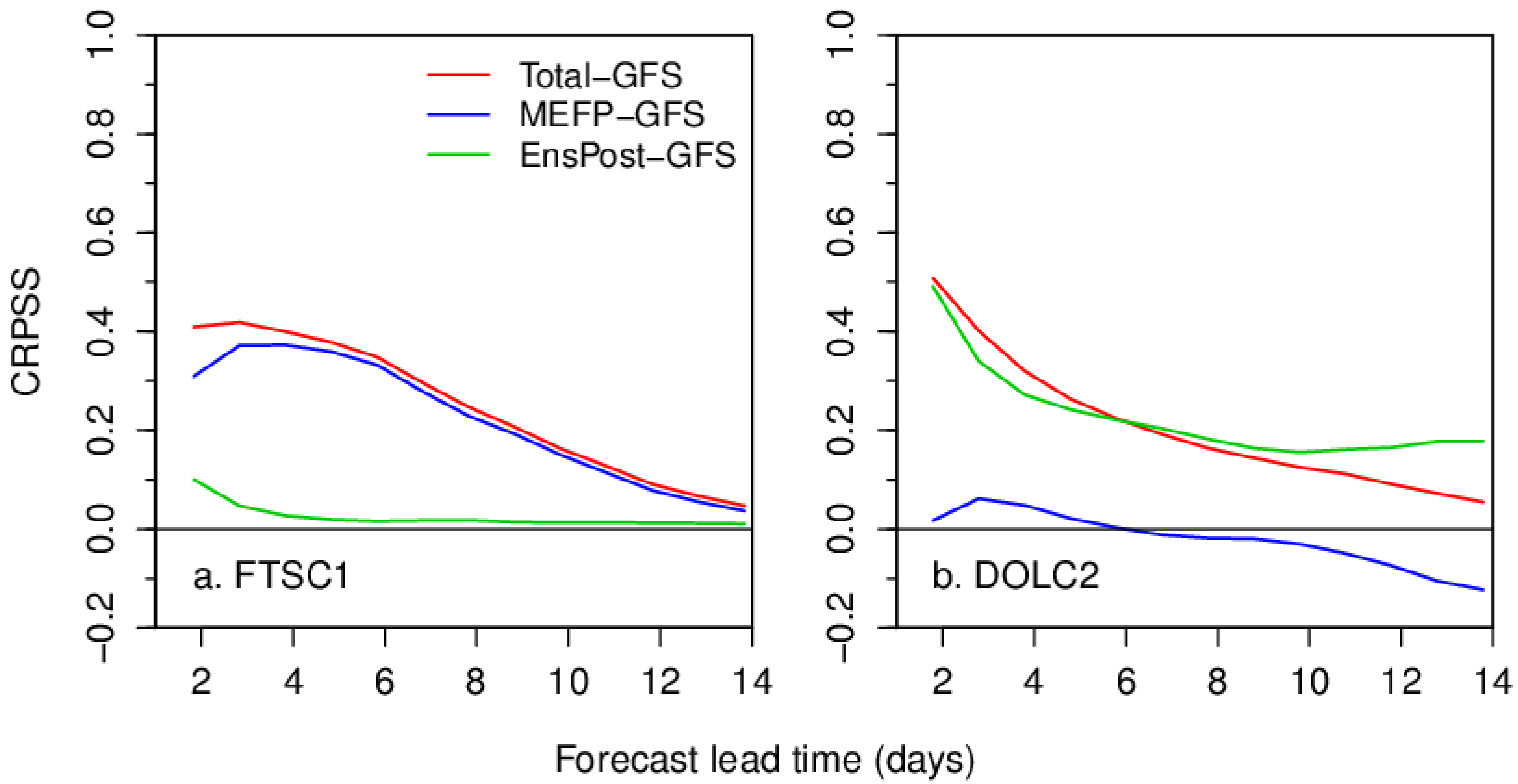
1. Meteorological forecast uncertainties
2. Hydrologic modeling uncertainties

- Can be further separated into many detailed sources

How do they contribute?

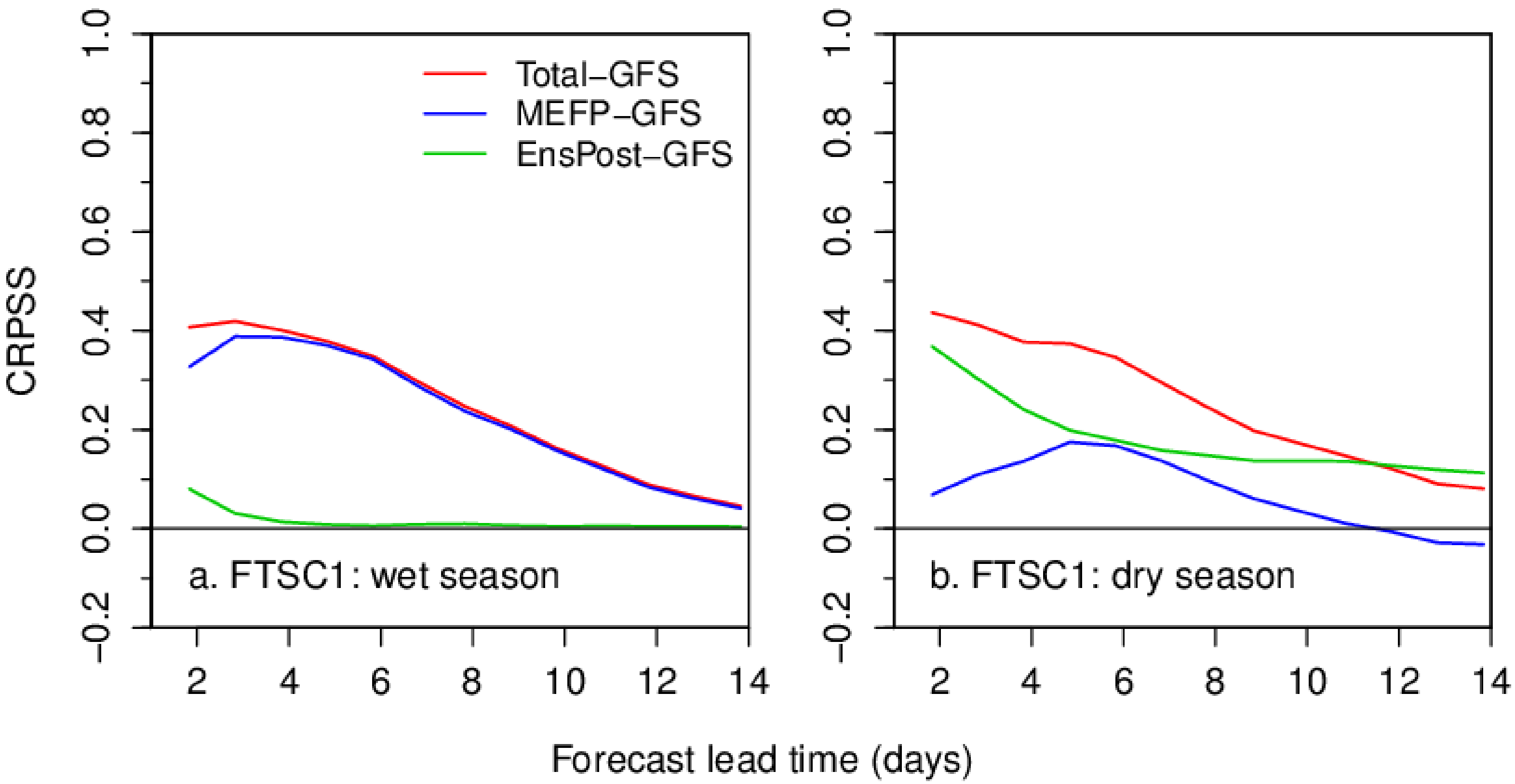
- Absolute and relative contributions vary considerably
- Data/model factors: forecast horizon, calibration etc.
- Physical factors: climate, location, season etc.

Example: two very different basins



- Fort Seward, CA (FTSC1) and Dolores, CO (DOSC1)
- Total skill in EnsPost-adjusted GFS streamflow forecasts is similar
- Origins are completely different (FTSC1=forcing, DOLC2=flow)

Example: two very different seasons



- However, in FTSC1, completely different picture in wet vs. dry season
- In wet season (which dominates overall results), mainly MEFP skill
- In dry season, skill mainly originates from EnsPost (persistence)

How do sources contribute?

Uncertainty in model output depends on

1. **Magnitude** of uncertainty in input sources
2. **Sensitivity** of the output variable to uncertain inputs

- Uncertainty in outputs increases with both factors
- Sensitivity is controlled by the model equations

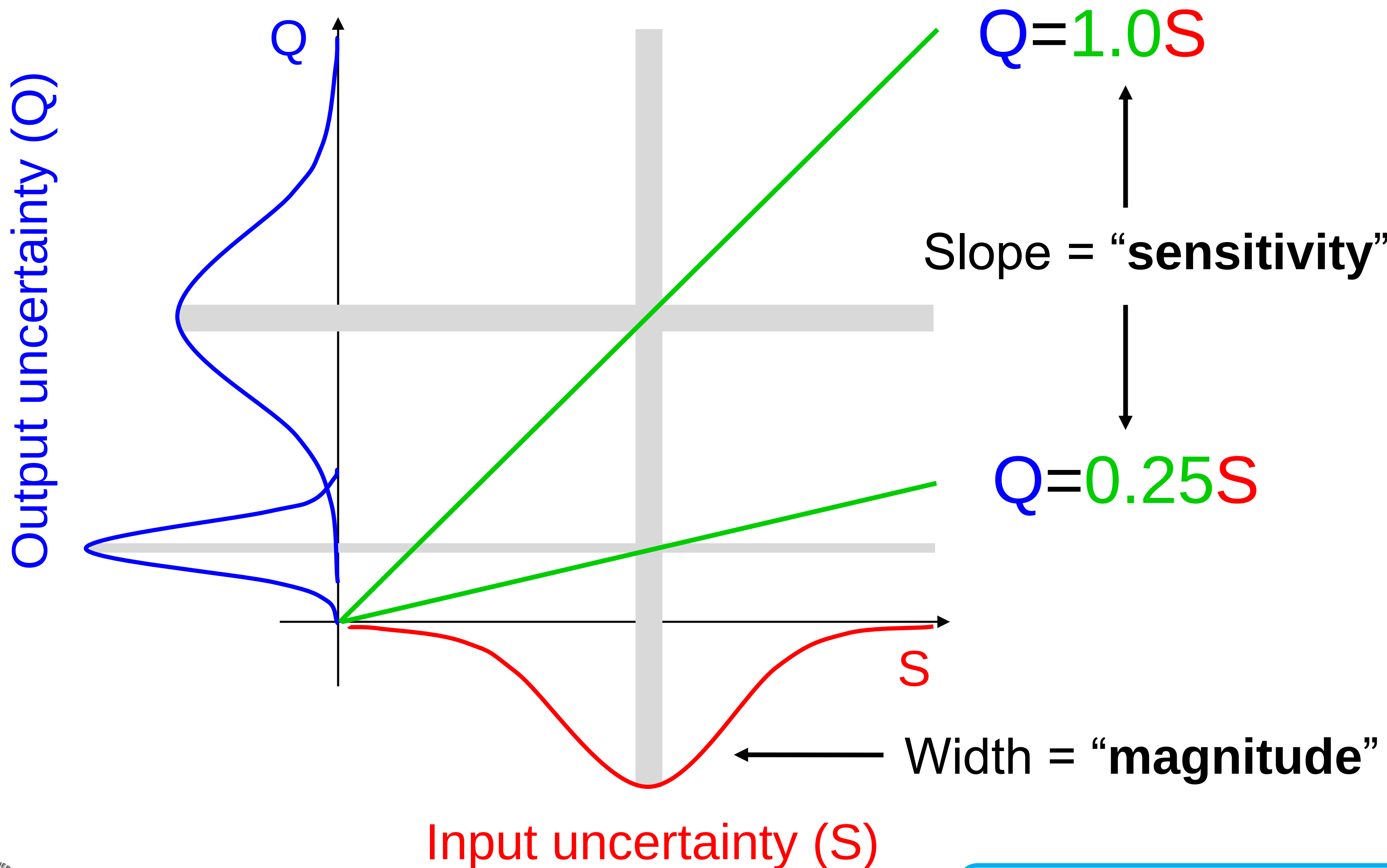
Simple example (one uncertainty source)

- Linear reservoir model, with flow equation:

$Q = wS$

Outflow = watershed coefficient * Storage

How do sources contribute?



How can we capture all sources?

What about non-hydrologic sources?

- Hydrologic outputs often used in additional models
- Are those uncertainties being considered?
- What about social and economic uncertainties?

What constitutes a “source”?

- Where to stop? Can always drill down further
- Detailed model may be desirable, but rarely practical
- Aggregate detailed sources, capturing total uncertainty
- For example: meteorological (S1) + hydrologic (S2)

Question 2: check all that apply

Flow forecast uncertainty depends on:

- ☐ A. Hydrologic uncertainty
- ☐ B. Meteorological uncertainty
- ☐ C. Magnitude of input uncertainties
- ☐ D. Economic and social uncertainties
- ☐ E. Basin characteristics
- ☐ F. Sensitivity of model output to each input

- Answers are at the end.

3. How to quantify the input sources of uncertainty?

Preliminaries: terminology

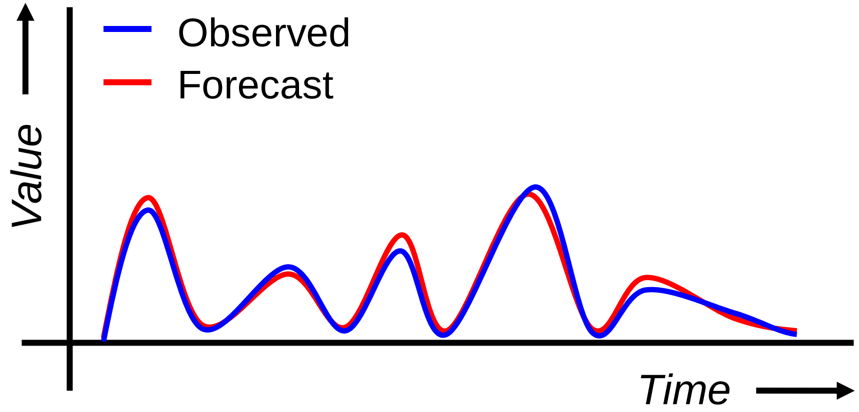
Error, bias, association

- Error: deviation between predicted and "true" outcome
- Bias: a consistent error (in one direction)
- Association: strength of relationship (ignoring bias)

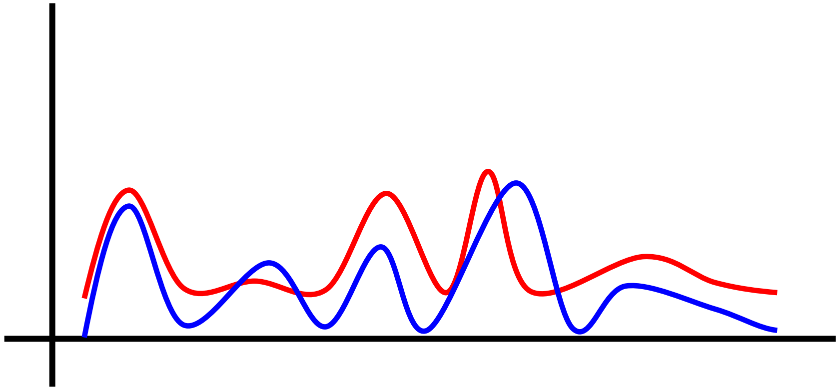
Uncertainty

- Inability to identify single ("true") outcome
- Equivalently: the inability to identify true error
- Randomness/unpredictability introduces uncertainty
- Need to model the possible errors (uncertainty)

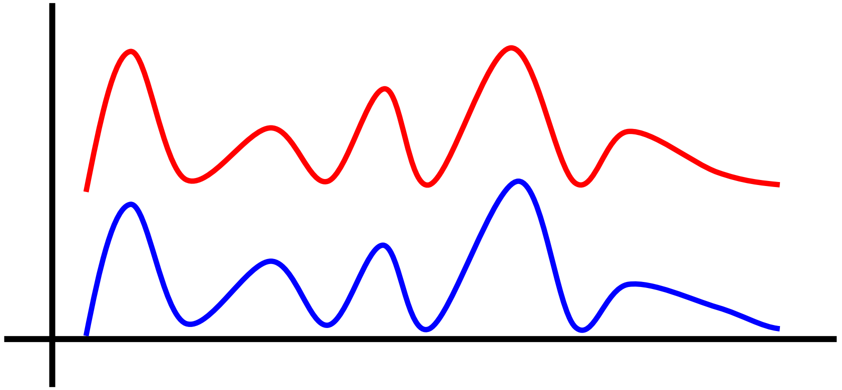
Error, bias, association



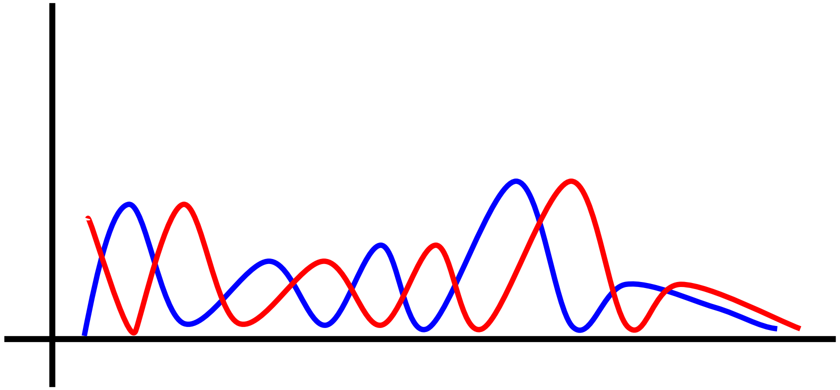
- Unbiased
- Strong association
- Small total error



- Some bias
- Moderate association
- Moderate total error

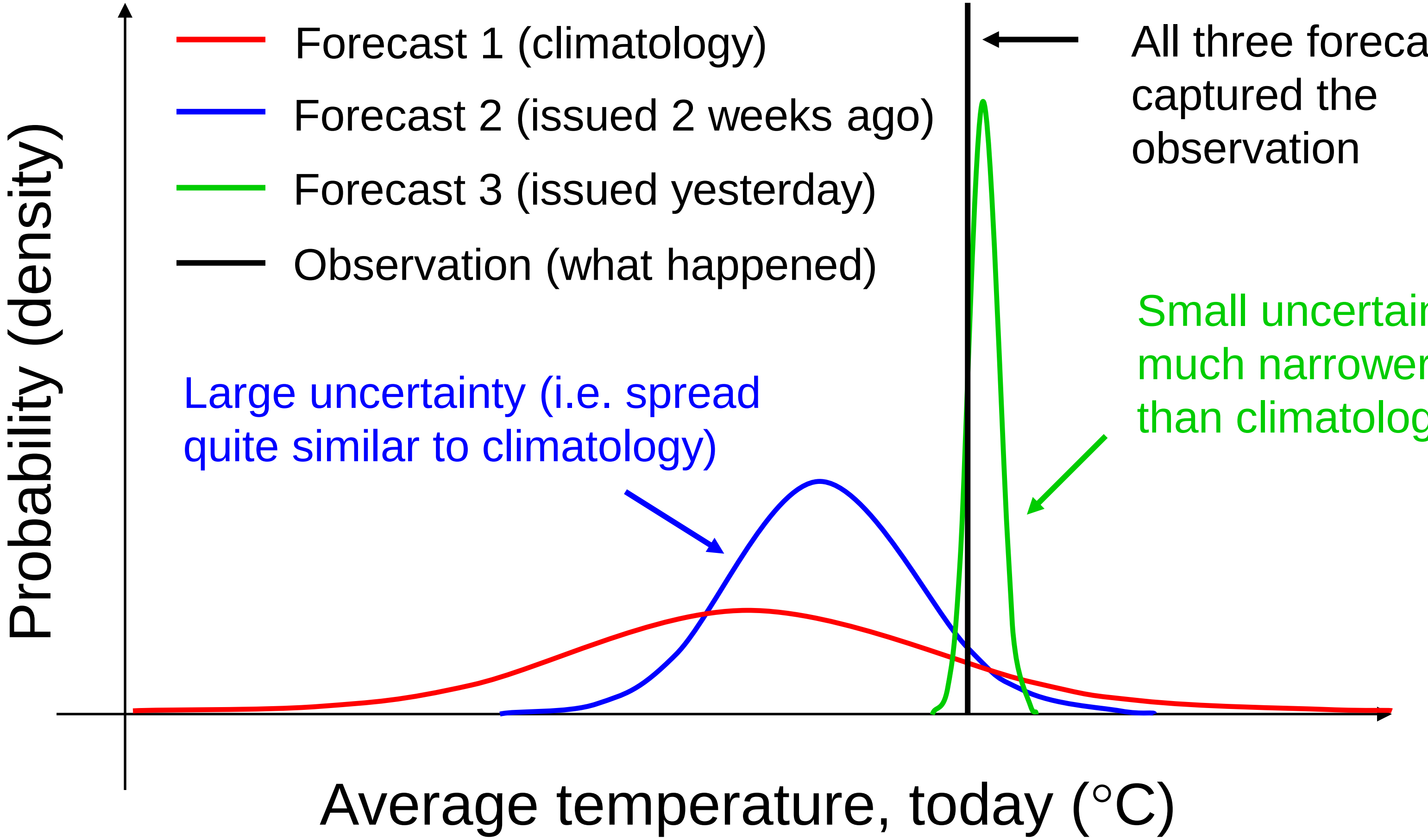


- Large bias
- Strong association
- High total error

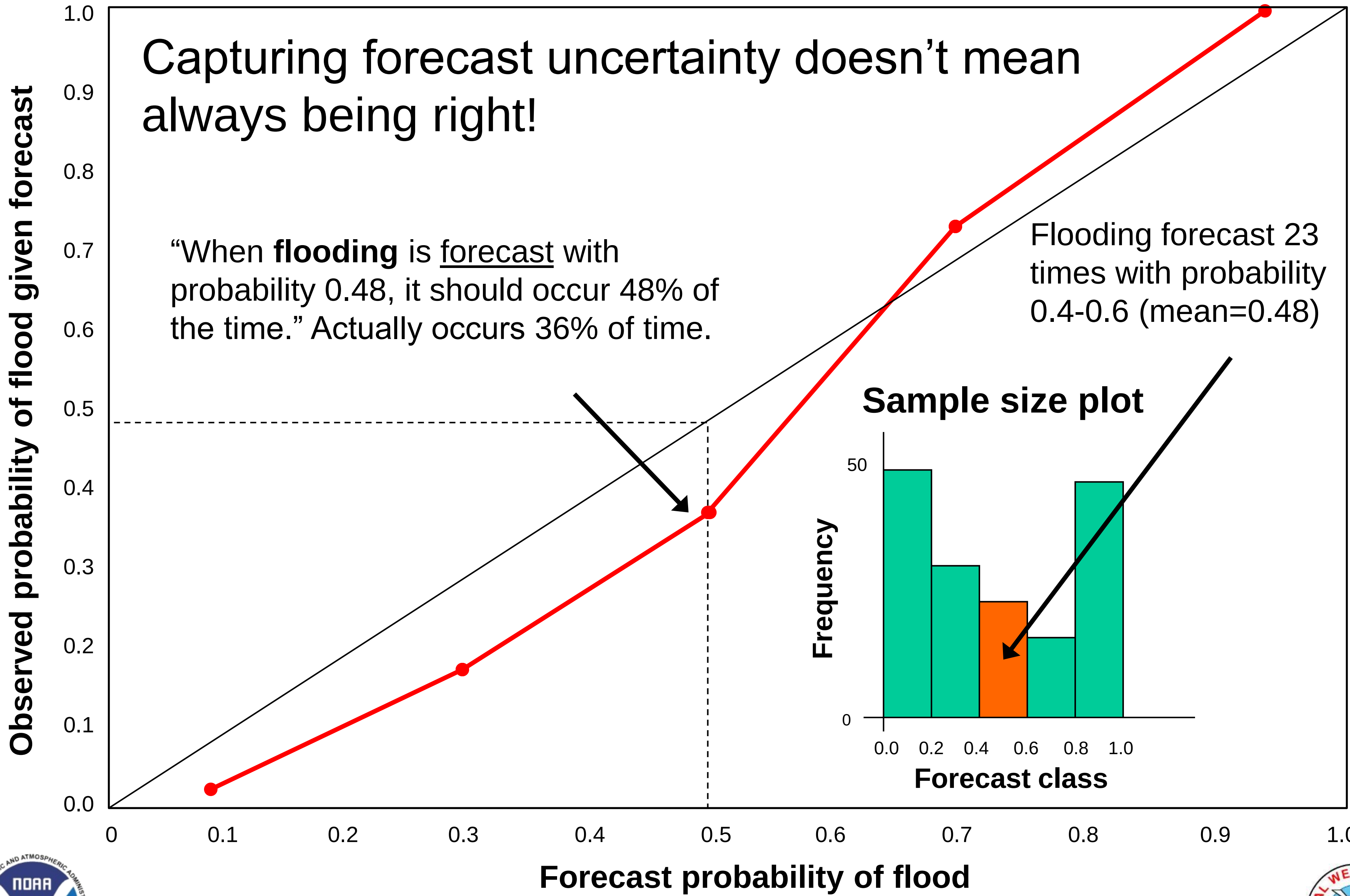


- Unbiased (but conditionally biased)
- Negative association
- High total error

Uncertainty is a relative quantity



Uncertainty: range can be wrong!



Foundations: random variables

What is a random variable?

- A variable with several possible outcomes
- Actual outcome is unknown (e.g. until observed)
- Event is a subset of outcomes (e.g. flows > flood flow)
- Strict rules for assigning probabilities to events

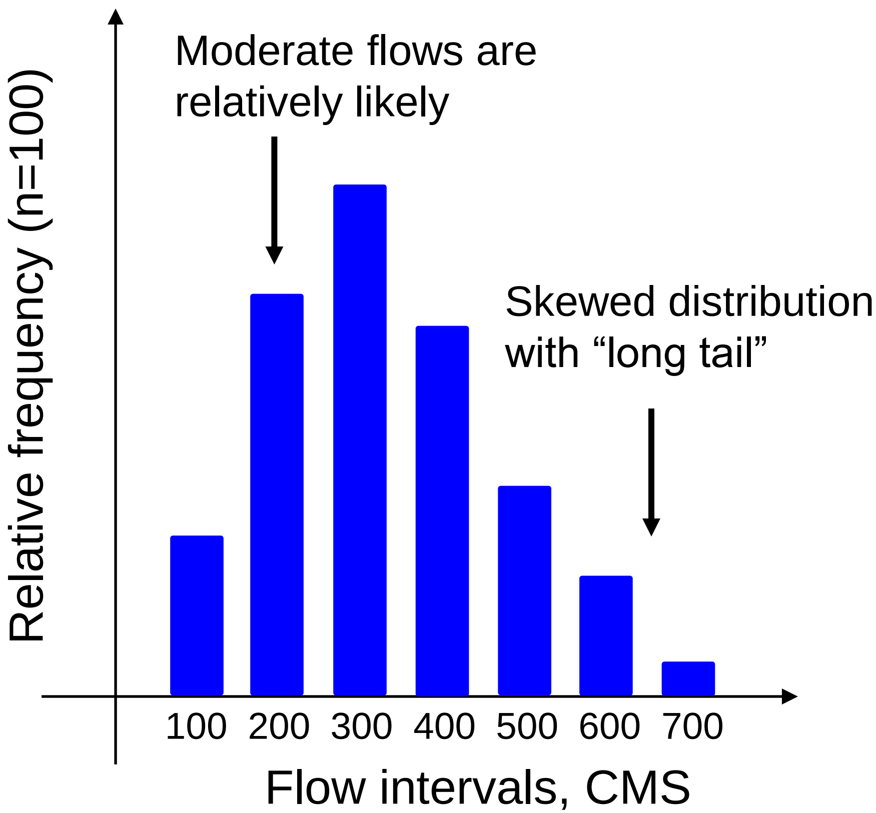
Types of (random) variable

1. **Continuous** (e.g. temperature)
2. **Discrete** (e.g. occurrence of a flood)
3. **Mainly continuous** (e.g. precipitation, streamflow)

SC.63-SC.65

Empirical approach

- Observe several (n) past outcomes, tabulate their relative frequencies, and plot histogram
- Useful for understanding climatological probabilities. Indeed, this is used for ESP
- But, limited to what happened in the past. Also, sample size dependent / noisy
- Thus, data often used to help calibrate a model for the probabilities in future. In other words, we use data in a model



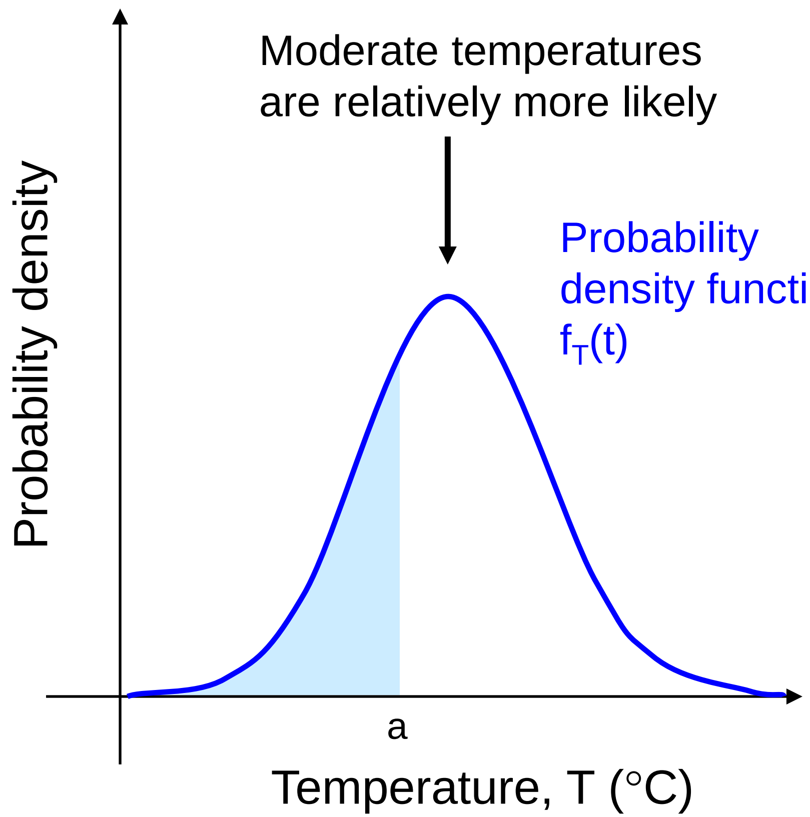
Interval	Frequency	Relative freq
100	4	4/100
200	15	15/100
…	…	…

4. The ingredients of a probability model

Probability density

PDF

- Applies to continuous variables only (e.g. temperature, flow)
- For continuous variables, probability is defined over an interval. For exact values, the interval is zero, hence Pr=0
- “Probability density function” (PDF) plots the concentration of probability within a tiny interval (infinitely small)
- Probability density must not be confused with probability. For example, densities can exceed 1



$$\Pr[T \le a] = \int_{-\infty}^{a} f_T(t)dt$$

Cumulative probability

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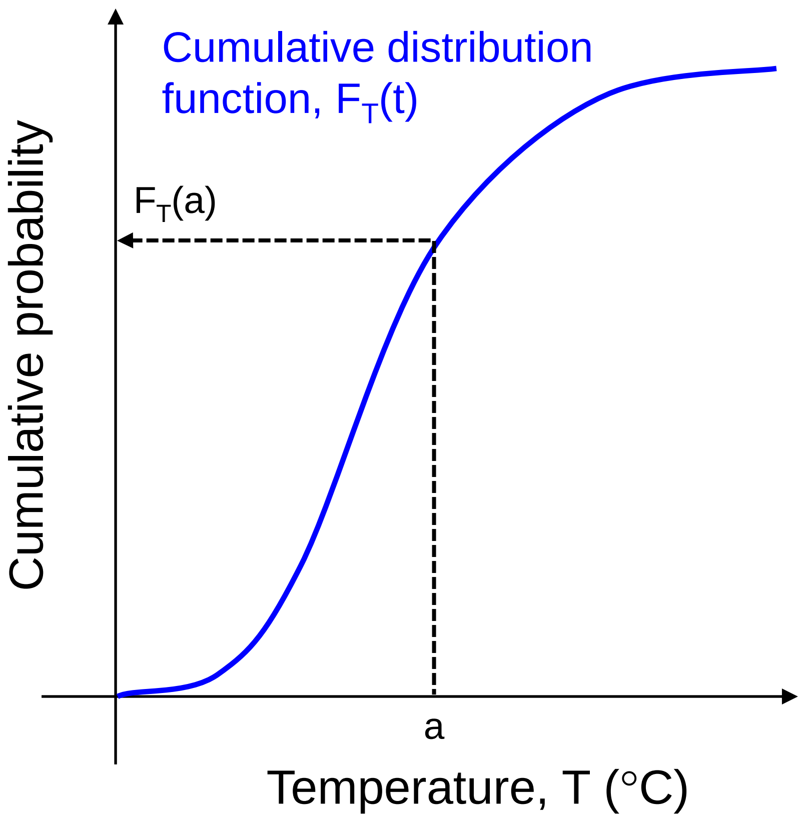
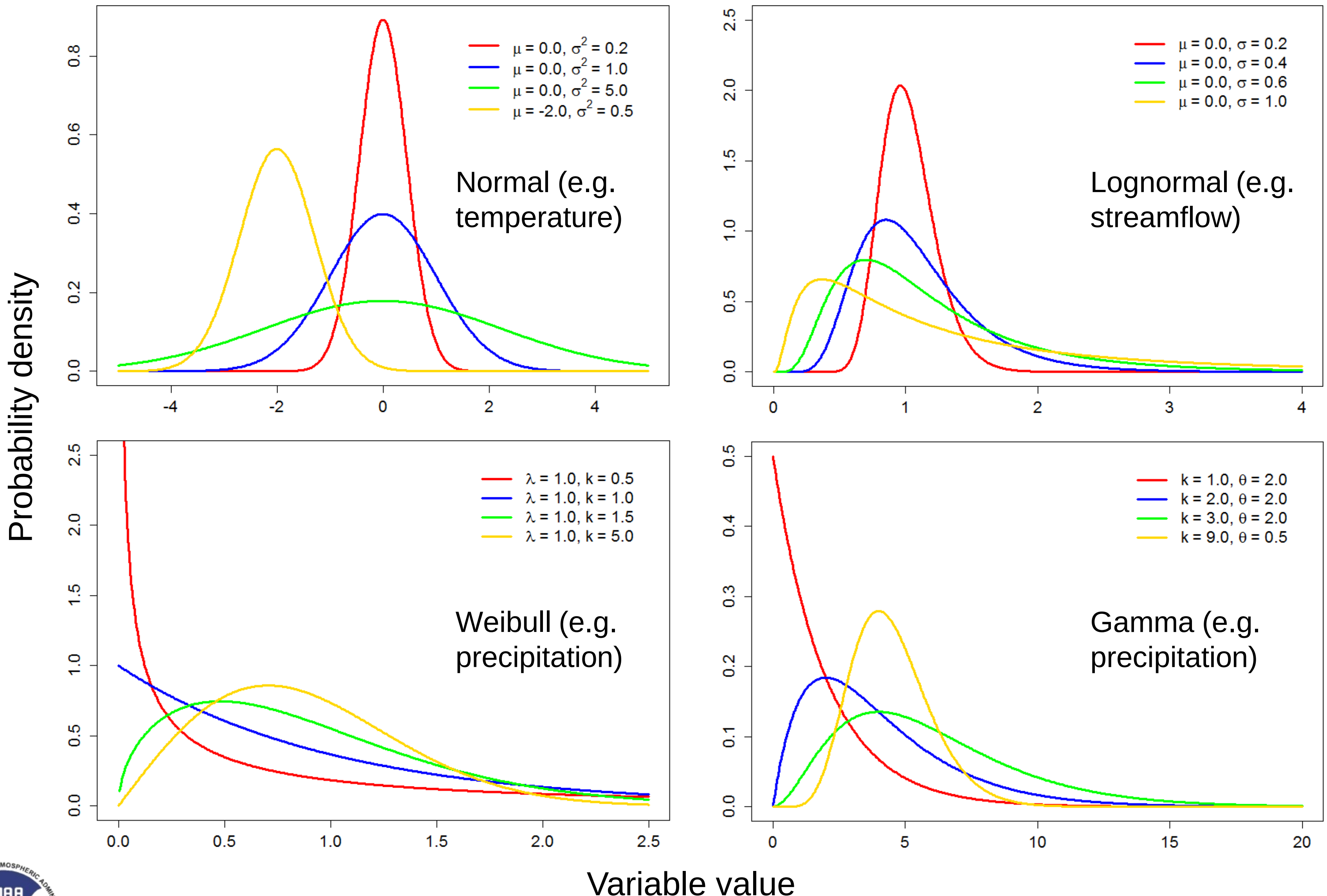
CDF

- Cumulative probability is the probability that the random variable takes a value less than or equal to the specified value
- Plotted for all possible values as a “cumulative distribution function” or CDF
- Cumulative probabilities are always between [0,1] and approach 0 at -∞ and 1 at +∞
- Cumulative probabilities are non-decreasing from left to right



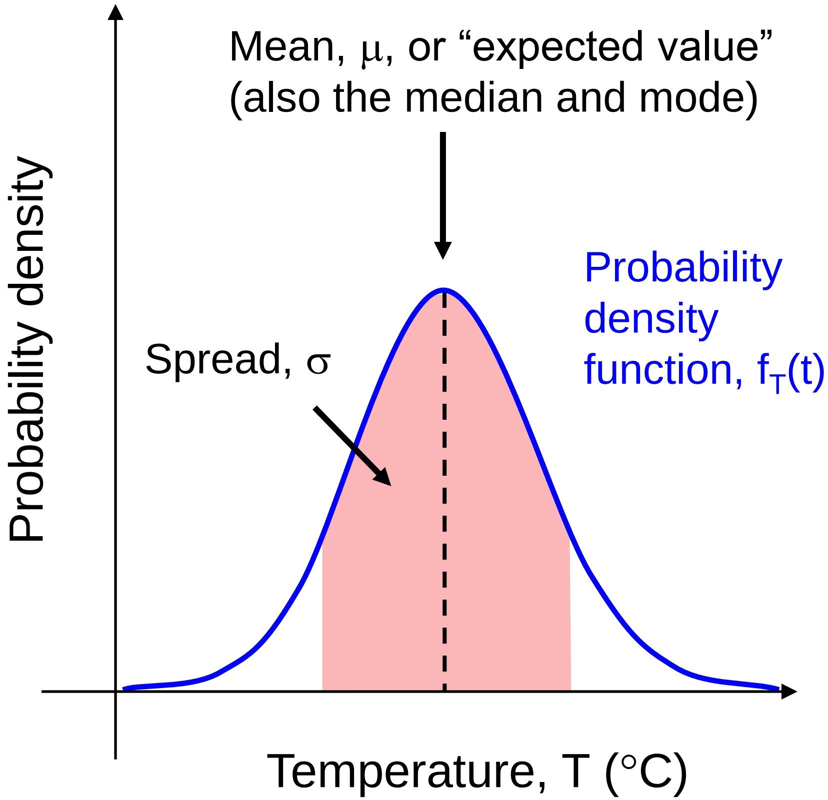
$$\Pr[T \le a] = F_T(a) = \int_{-\infty}^{a} f_T(t)dt$$

Some common PDFs



A common shape

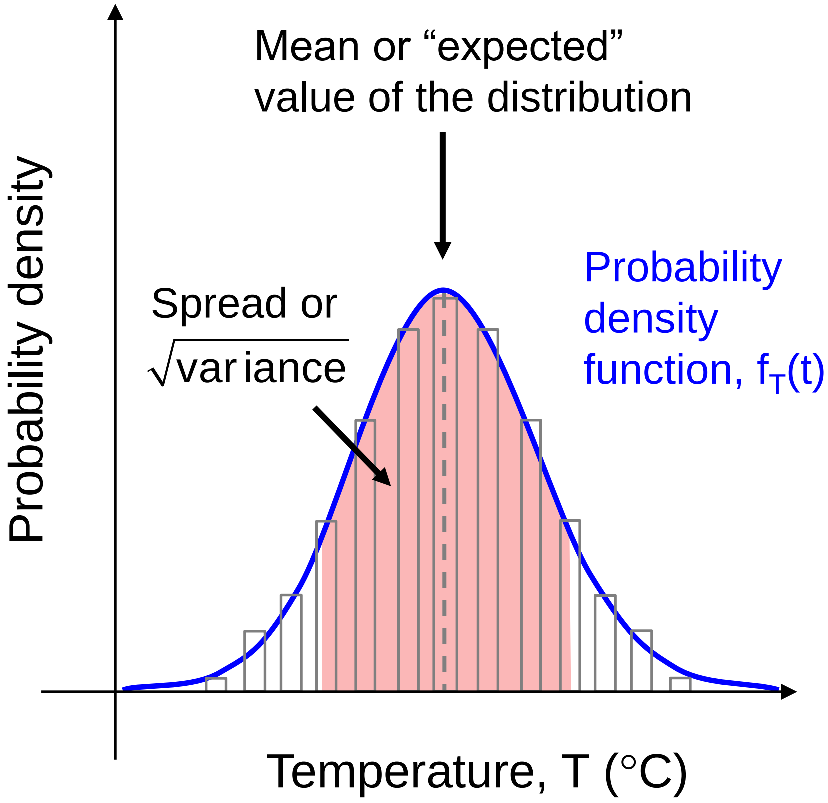
- **Central Limit Theorem:** under certain (common) conditions, a sum of random variables is approximately normal
- Sums of random variables are common in nature & engineering
- Thus, many variables are approx. normally distributed
- Normal is a simple shape with many desirable characteristics…
- E.g. A linear combination of normal variables is also normal!



$$f_T(t) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(t-\mu)^2}{2\sigma^2}}$$

Model parameters

- Fitted probability distributions have parameters to estimate
- Parameters dictate location, width, precise shape etc.
- Normal distribution is specified by the mean and spread
- Different ways to estimate parameters. For example, using historical sample data (right)
- When forecasting a random variable, the future parameters depend on the <u>forecast model</u>



$$\text{mean} \approx \frac{1}{n}\sum_{i=1}^{n} t_i$$

$$\text{variance} \approx \frac{1}{n}\sum_{i=1}^{n} (t_i - \text{mean})^2$$

Question 3: check <u>all</u> that apply

The normal distribution is:

- ☐ A. A skewed probability distribution
- ☐ B. Completely defined by its mean value
- ☐ C. Symmetric
- ☐ D. A distribution with equal mean, median and mode
- ☐ E. Widely used in probability and statistics
- ☐ F. Applicable to discrete random variables

- Answers are at the end.

Marginal & conditional probability

Marginal probability

- Simplest case, involving one random variable
- For example, streamflow at one time and location
- Can be expressed as a PDF or CDF (see above)

Conditional probability

- A probability distribution that is subject to conditions
- For example, streamflow given that precipitation > 0
- This is expressed as a (conditional) PDF or CDF
- We express these conditions if they are important

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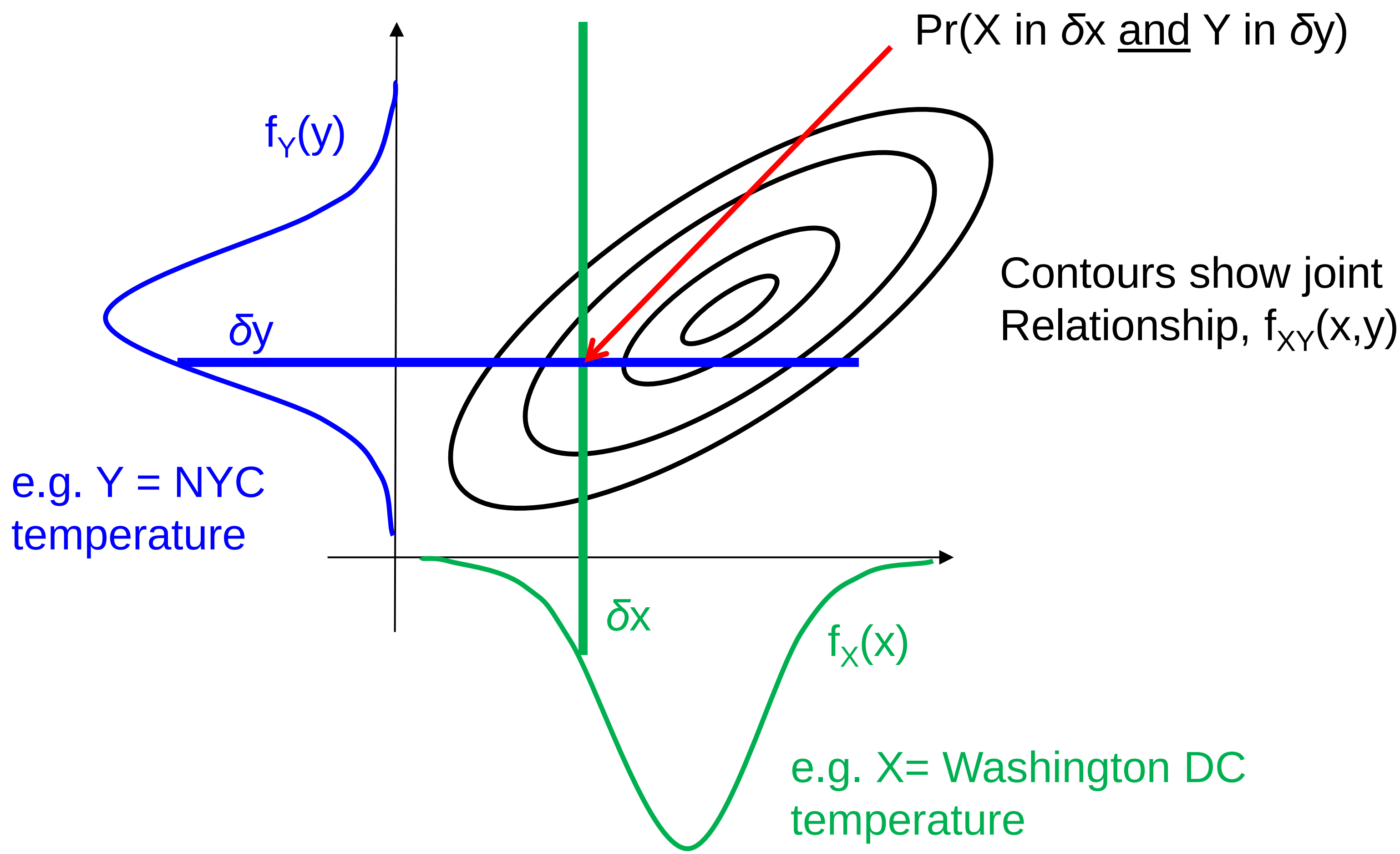
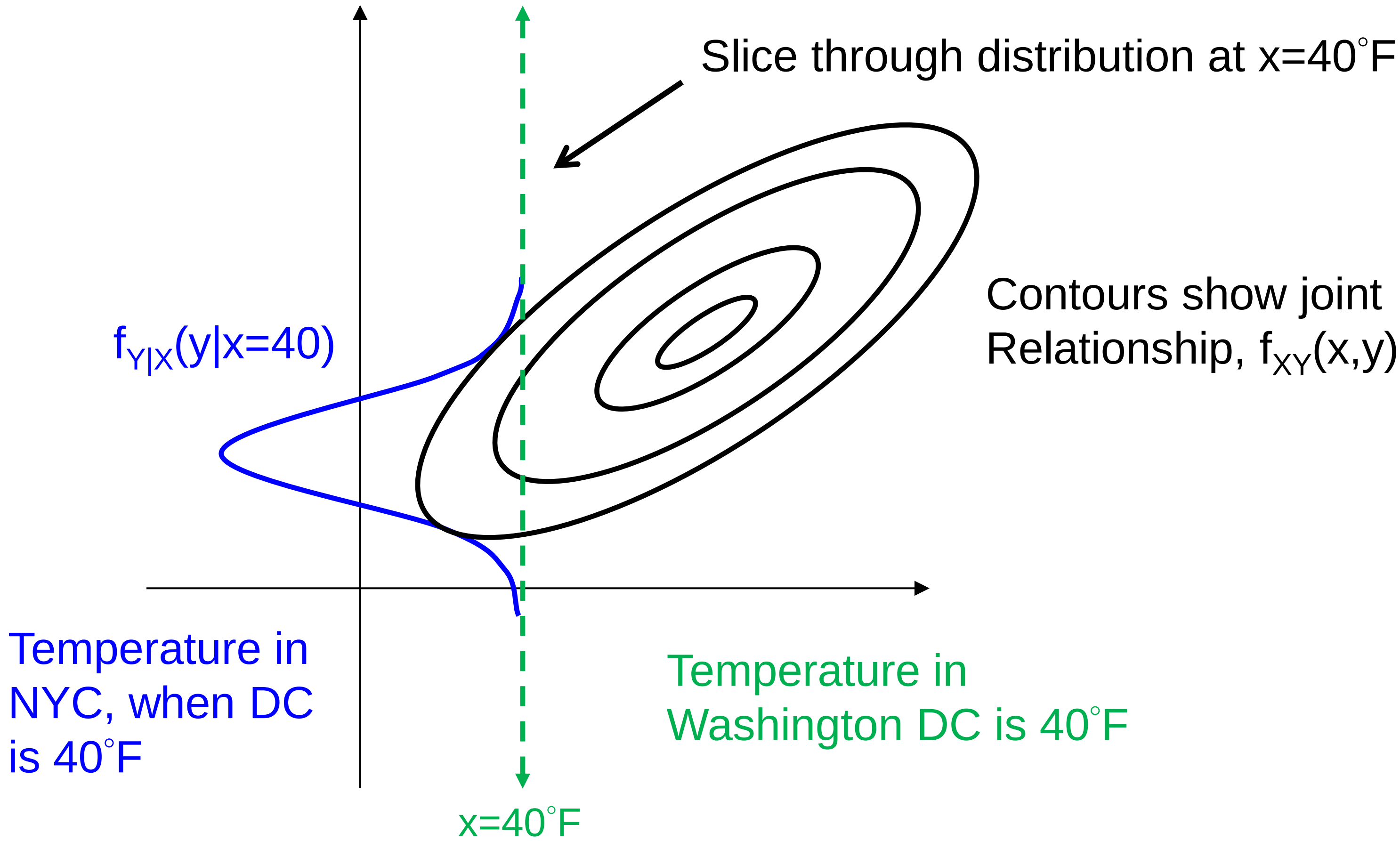
Two random variables (could be more)



Contains marginals and conditionals



Joint probability distribution

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What does it tell us?

- Contains information about each variable (marginals)
- Contains information about how they are related
- Could involve multiple times, locations, variables,…

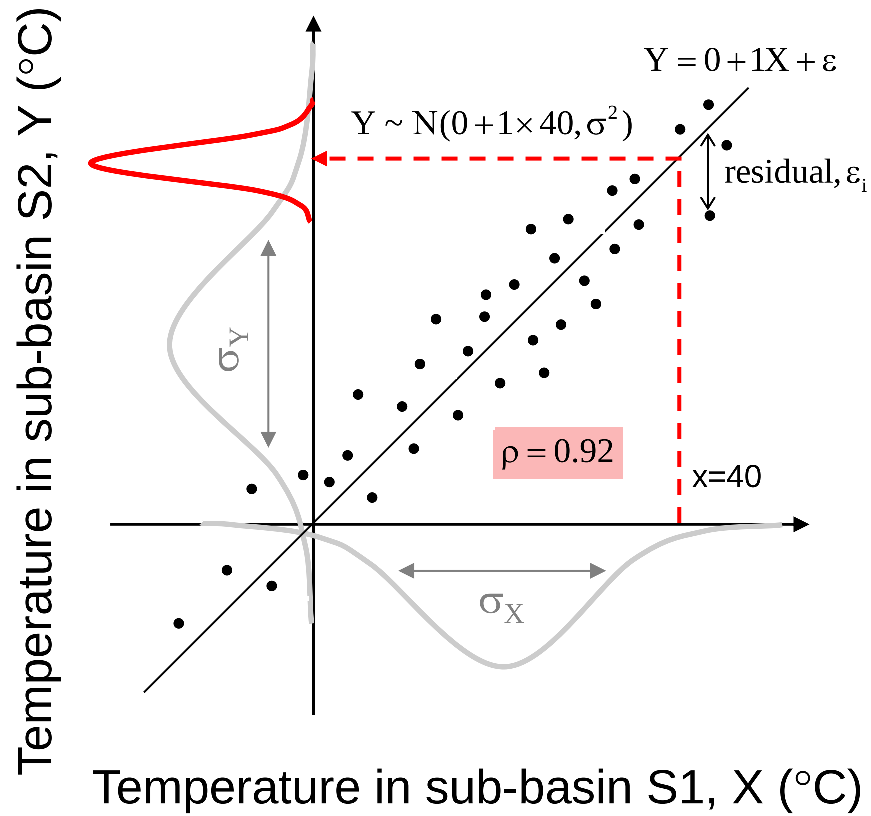
Why do we need to consider this?

- Hydrologic models have inputs that are dependent
- For example, temperature, precipitation, evaporation
- Can't have "snow" ensemble member at 40°C!
- Many different ways to model this dependence

Linear dependence and correlation

Correlation, ρ

- Measures degree of linear (not non-linear!) association between two continuous variables, X & Y
- For two joint normally distributed variables, correlation captures their joint relationship
- Linear modeling is common in hydrometeorology. Thus, correlation is widely used
- If input (X) to a linear regression is normal, output (Y) is normal (N) with mean, $\alpha+\beta X$, and variance (σ^2) equal to variance of residual, ε



$$Y = \alpha + \beta X + \varepsilon$$

$$\beta = \rho \frac{\sigma_Y}{\sigma_X}, \varepsilon \sim \text{Normal}(0, \sigma^2)$$

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Data transforms are common

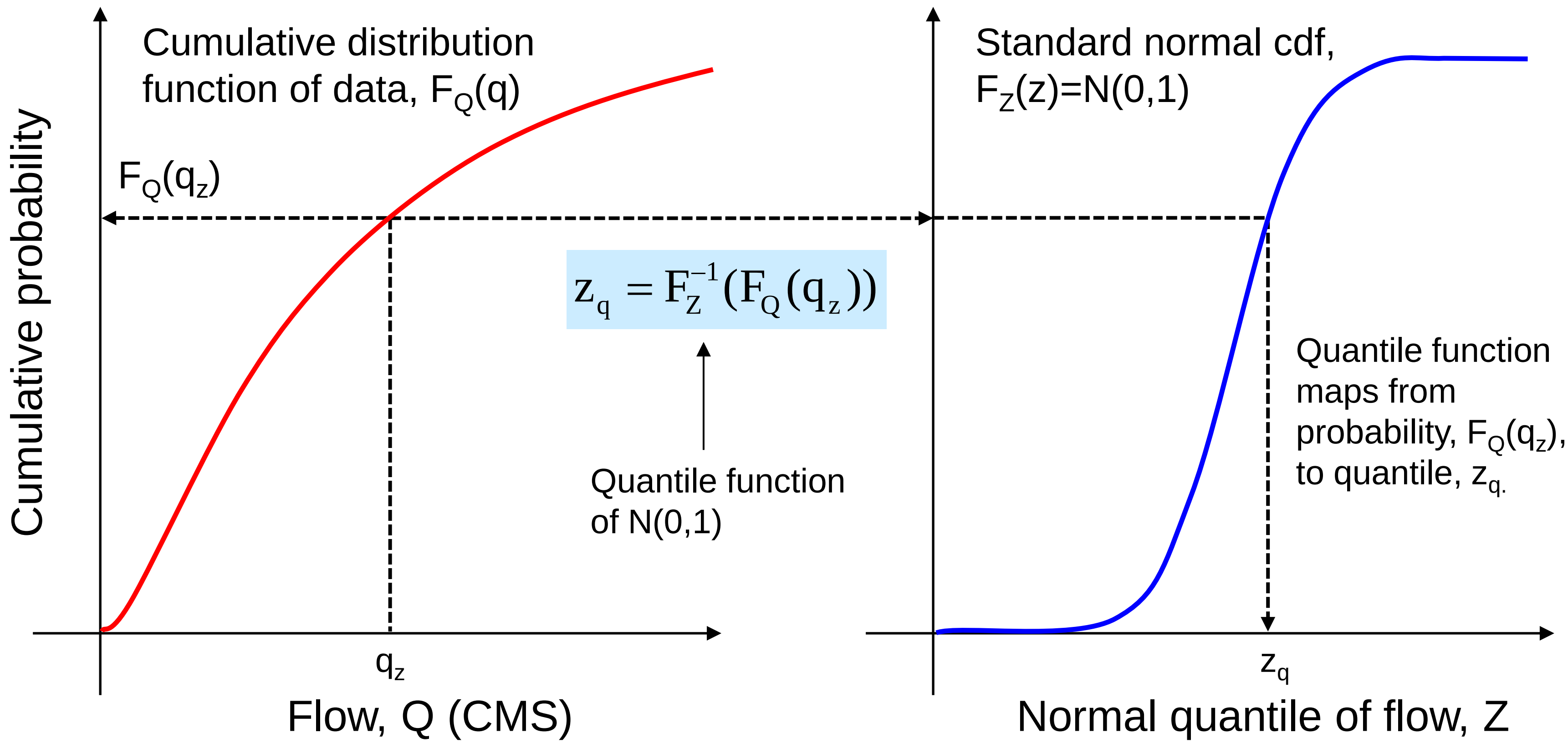
- Many reasons for data transforms
- For example, to suppress extreme values
- Power transforms widely used (e.g. Box-Cox)
- Often used to make data more normally distributed

Distribution remapping

- More aggressive, non-linear, data transformation
- Maps distribution of Q to a standard distribution, Z
- Normal Quantile Transform (NQT) is one example…

Normal Quantile Transform (NQT)

Transform data to be marginally normal



- Need to back-transform each model prediction to flow space

Modeling considerations

When theory meets hydrologic reality

- Variables often highly skewed, strongly not normal
- Space/time and cross-variable relations are complex
- Climate/river processes can change (non-stationarity)
- Sub-populations often exist (e.g. amount-dependence)

What is the optimal model complexity?

- Keep it simple: what can reasonably be ignored?
- Limited historical data implies a simpler model…
- …otherwise, there's a real risk of "curve fitting"

Question 4: check all that apply

The correlation coefficient is:

- ☐ A. A parameter of the bivariate normal distribution
- ☐ B. A parameter of the marginal normal pdf
- ☐ C. Always zero for two independent variables
- ☐ D. Rarely applicable
- ☐ E. A measure of linear dependence
- ☐ F. A measure of non-linear dependence

- Answers are at the end.

5. How to quantify the output (i.e. forecast) uncertainty?

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Foundation for ensemble prediction

- For <u>any</u> model, g, with inputs $\{X_{1,\ldots,}X_m\}$ and output, Y:

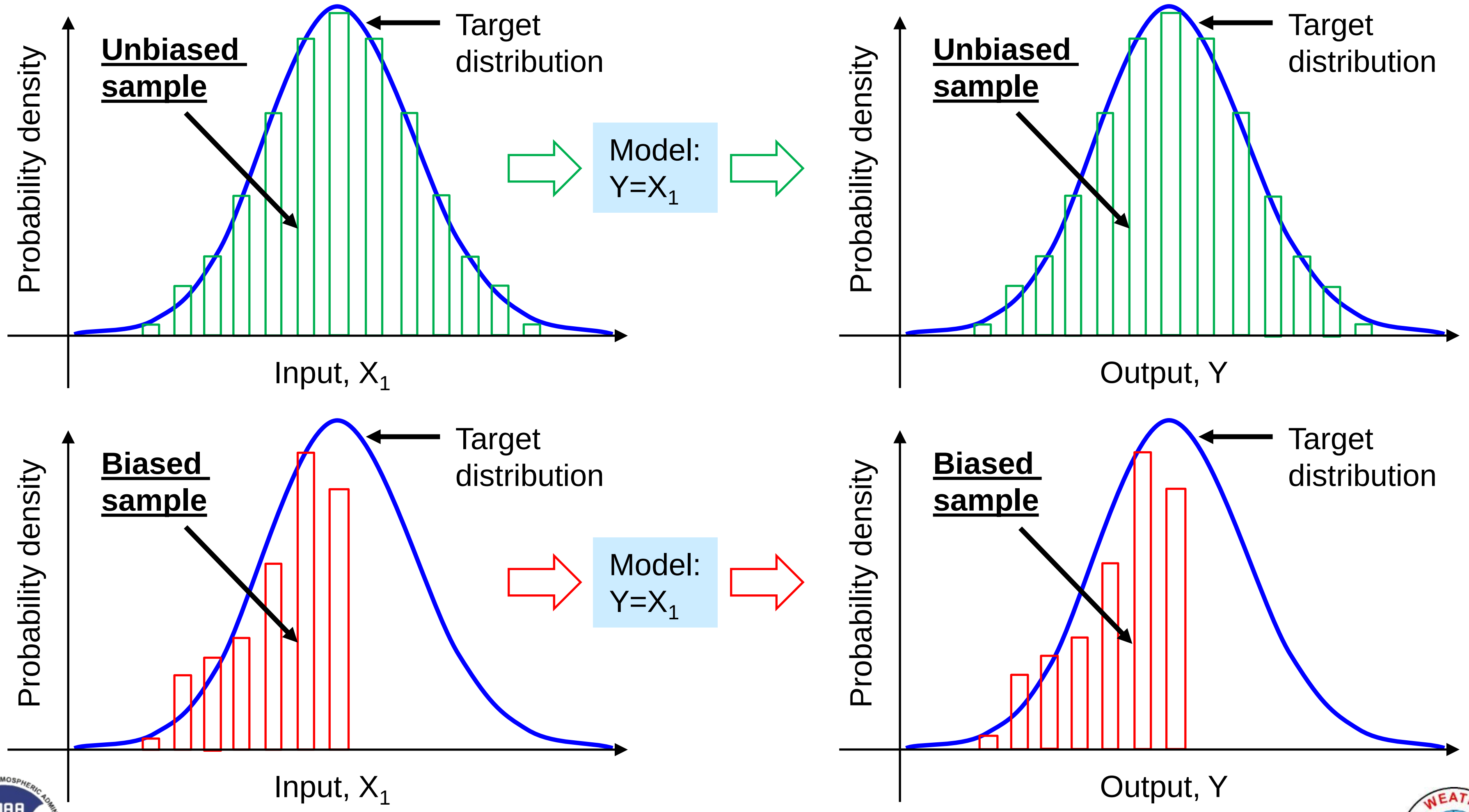
1. Draw a random sample, $\{x_{1,\ldots,}x_m\}$, from input joint PDF
2. Run the model, $y_1=g(x_{1,\ldots,}x_m)$, and store the result
3. Repeat n times (e.g. n=1000) or until PDF of Y is stable

Scales up with model complexity

- Makes no assumptions about g: just a “black box”
- Thus, works for complex, non-linear, models
- As accurate as required (i.e. $n \rightarrow \infty$), but runtime high!

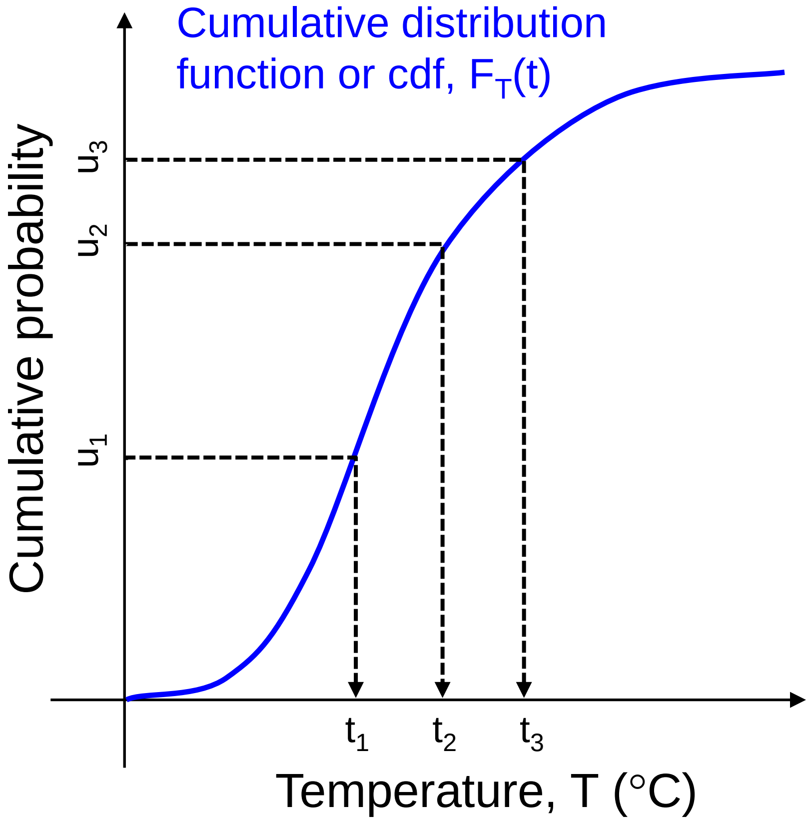
Importance of unbiased sampling

Each sample must be equally likely!



Sampling any CDF

- Many different approaches to random sampling, depending on probability distribution
- Simplest, generic, approach is “inverse transform sampling”
- Start with a standard Uniform distribution, U(0,1)
- Any pseudo-random number generator samples from U(0,1)
- For random sample, $u_1,\ldots,u_n$, transform numbers to target distribution, $F_T(t)$, as $t_i = F_T^{-1}(u_i)$



$$t_i = F_T^{-1}(u_i)$$

Question 5: check all that apply

Monte Carlo simulation requires:

- ☐ A. A simple forecast model
- ☐ B. An equal chance of sampling each possible value
- ☐ C. The joint probability distribution of model inputs
- ☐ D. Uncorrelated inputs
- ☐ E. Running the forecast model many (n) times
- ☐ F. An infinitely large sample size

- Answers are at the end.

6. Applying the theory to operational forecasting in hydrology

Reminder of uncertainty sources

Total uncertainty in streamflow from:

1. Meteorological forecast uncertainties
2. Hydrologic modeling uncertainties

- (But don't forget social/economic/decision context)

Hydrologic uncertainties include

- Model structure (SNOW-17, SAC-SMA, Lag/K etc.)
- Model parameters
- Initial conditions and state variables
- River regulations, reservoirs, manual adjustments

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Different techniques and aims

- Broadly speaking, two groups of techniques:

1. Those that do **not** aim to quantify total uncertainty
   - Risky. Generally, they ignore hydrologic uncertainties
2. Those that do aim to quantify total uncertainty
   a. By modeling directly (statistically) in a lumped way (also known as Model Output Statistics, MOS)
   b. By modeling indirectly, via individual sources (i.e. by conducting uncertainty propagation)
   c. Extension of b. to remove biases in forcing and/or flow

Examples of operational techniques

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Characteristics of selected systems

Characteristic	US-ESP	US-MMEFS	US-HMOS	US-HEFS	EU-EFAS
Models total uncertainty	✗	✗	✓	✓	✓
Models met. uncertainty	✓	✓	✗	✓	✓
Models hydro. uncertainty	✗	✗	✗	✓	✓
• Parameter uncertainty	✗	✗	✗	✗	✗
• Structure uncertainty	✗	✗	✗	✗	✗
• State updating	✗	✗	✗	✗	✗
Corrects overall streamflow bias	✗	✗	✓	✓	✓
Corrects met. bias (pre-proc.)	✗	✗	✗	✓	✗
Corrects hydro. bias (post-proc.)	✗	✗	✗	✓	✗
Uses single-valued forcing	✗	✗	✓	✓	✗
Uses full ensemble forcing	✗	✓	✗	✗	✓
Uses climatological forcing	✓	✗	✗	✓	✗
Provides short-range forecasts	✗	✓	✓	✓	✓
Provides medium-range forecasts	✗	✓	✓	✓	✓
Provides long-range forecasts	✗	✗	✗	✓	✗

HEFS concept

Aim: quantify total uncertainty in flow

Address two key uncertainty sources	STEP 1: model (“learn from past”)	STEP 2: forecast (“apply to future”)

Meteorological uncertainty

- Precipitation/temperature
- “Raw” forecasts
  - Short: **RFC, GEFS**
  - Medium: **GEFS**
  - Long: **CFSv2, climate**

→

MEFP model and parameter estimator

- Historical raw forecasts
- Historical observations
- Model uncertainty/bias
- Operates at basin-scale

→

MEFP forecaster

- Take raw input forecast
- Quantify unc./bias
- Sample members

→ Hydrologic models

Hydrologic uncertainty

- Model states
- Model parameters
- Model structure
  - SAC-SMA/SNOW17

→

EnsPost model and parameter estimator

- Lumped approach
- Historical simulations
- Historical observations
- Model uncertainty/bias

→

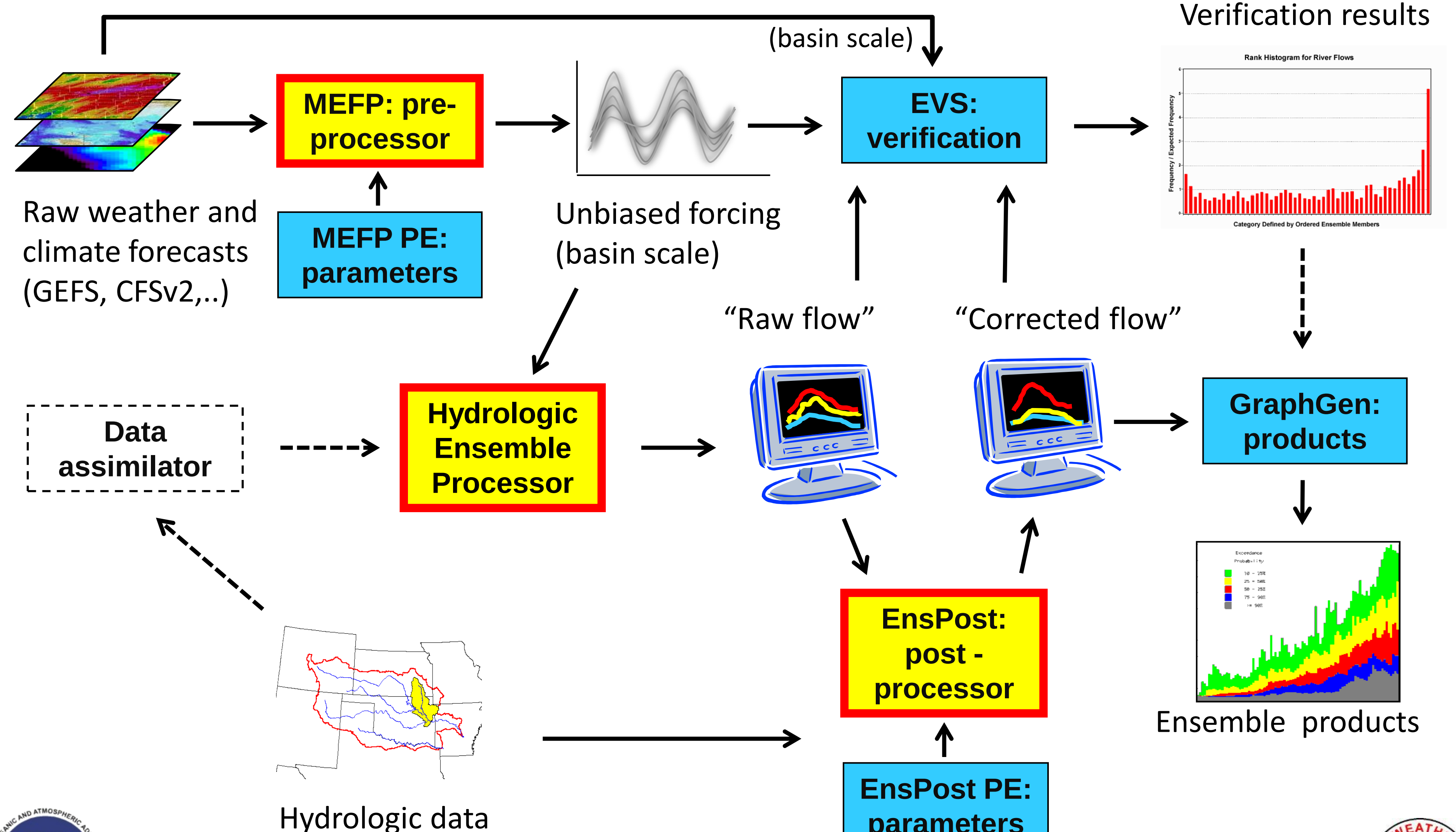
EnsPost forecaster (final HEFS forecast)

- Take simulation
- Quantify unc./bias
- Sample members
- Adjust “raw” flow

← Hydrologic models

HEFS software components

= Forecast tool (real-time/hindcast) = Supporting tool ---- = Future capability



Many challenges remain

Modeling challenges

- Accounting for all major sources of uncertainty
- Accounting for joint relationships (in space/time etc.)
- Accounting for real-time MODs and regulations
- Accounting for uncertainties beyond hydrology

Service challenges for operational use

- Ensuring continuity of service (e.g. w/ NCEP models)
- Ensuring adequate training for use of ensembles
- Communicating uncertainties broadly & successfully

Question 6: check all that apply

The NWS HEFS aims to:

- ☐ A. Quantify the total uncertainty in streamflow
- ☐ B. Quantify the meteorological uncertainties only
- ☐ C. Correct for biases in the streamflow forecasts
- ☐ D. Avoid the need for hydrologic model calibration
- ☐ E. Produce equally likely traces of streamflow
- ☐ F. Correct for biases in the meteorological forecasts

- Answers are at the end.

Resources and references

- Hydrologic Ensemble Prediction Experiment (HEPEX). Visit www.hepex.org
  - E.g. http://hepex.irstea.fr/operational-heps-systems-around-the-globe/
- HEFS documentation: http://www.nws.noaa.gov/oh/hrl/general/indexdoc.htm

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Advanced slides and answers to questions

Advanced slides from Section 2

Generalizing to additional sources

Output uncertainty (in simplest case)

- Linear model, g, uncorrelated inputs, X_i, output, Y

$$\mathrm{Var}(Y) = \sum_{i=1}^{m} \mathrm{Var}(X_i) \cdot \left(\frac{\partial g}{\partial X_i} \right)^2$$

Here, the variance (Var) is a measure of "average uncertainty". The derivative is the "slope" for input X_i, which is the sensitivity.

- Output unc. = (sum of) input unc. * input sensitivity

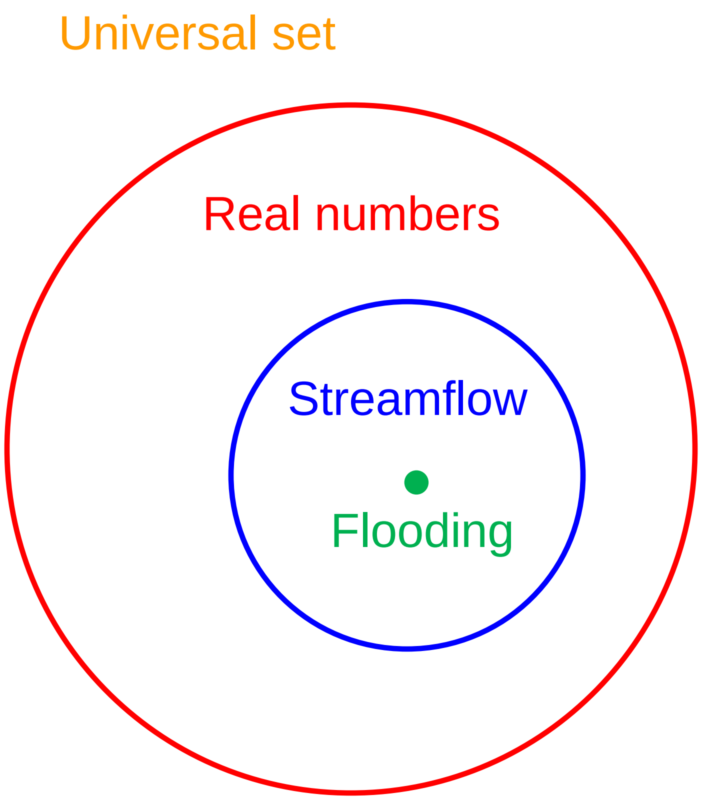
Simple equation, but rarely applicable

- Principle always applies (i.e. magnitude * sensitivity)
- But g is rarely linear and inputs rarely uncorrelated
- For hydrologic models, need an ensemble approach

Advanced slides from Section 3

The sample space

- The **set** of all possible values or **"outcomes"** that a random variable could take (e.g. the possible values of streamflow)
- The universal set is the largest set (it contains everything)
- Streamflow is a subset of real numbers, i.e. no negative flows
- An **event** is a subset. It contains one or more possible outcomes (e.g. streamflow values)
- For example, flooding is an event (flow values > flood flow)



Question A1: check all that apply

A random variable is:

- ☐ A. The opposite of a deterministic variable
- ☐ B. A complete probabilistic description
- ☐ C. Streamflow
- ☐ D. A discrete event
- ☐ E. An uncertain variable
- ☐ F. A variable with a sample space of events

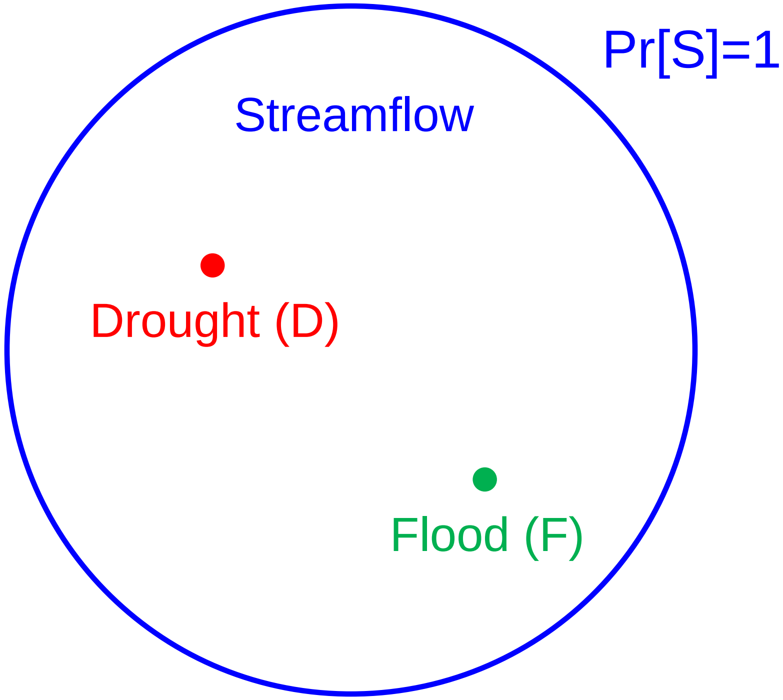
- Answers are at the end.

Probability measure

- Assigns a probability to every possible event, E, in the sample space, S
- A probability measure must follow certain logical rules or "axioms", namely:

1. Probabilities between [0,1]
2. Probabilities (Pr) of mutually exclusive events are additive: Pr[Drought or Flood] = Pr[Drought]+Pr[Flood]
3. Sum of all probabilities equals 1

$0 \leq Pr[E] \leq 1$ for all E



Pr[Drought or Flood]
= Pr[Drought]+Pr[Flood]

But how best to define a model?

Two schools of thought (big topic!)

- Two approaches to *using* probability laws

1. Frequentist approach emphasizes data (empirical)
2. Bayesian approach exploits all available knowledge

Modern Bayesian paradigm

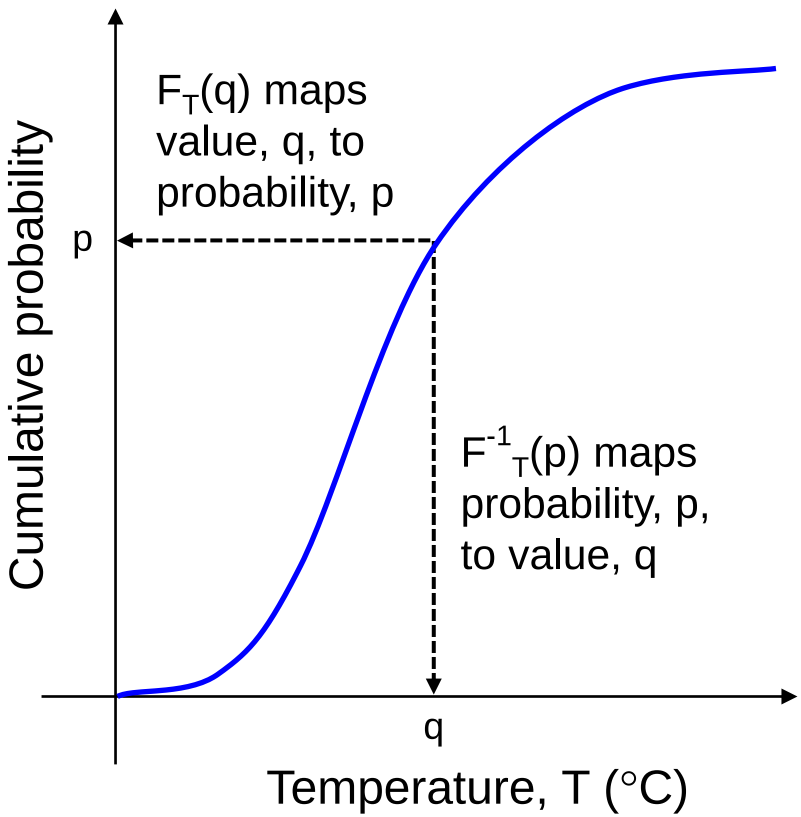
- Frequentist approach is too narrow/limiting…
- …rivers change (history not always applicable)
- …information about rivers changes (e.g. new dataset)
- Bayesians embrace data, models, expert opinions

Advanced slides from Section 4

HSL

Quantiles

- The CDF provides a mapping between real values and (non-exceedence) probabilities
- For a given probability, p, the corresponding real value, q, is known as the q-**quantile**
- For example, the median is the 0.5 quantile or the 50th percentile as 50% of values fall below this
- The inverse of a CDF is expressed as $F_T^{-1}(p)$ and is known as the "quantile function." Thus, the median is $F_T^{-1}(0.5)$

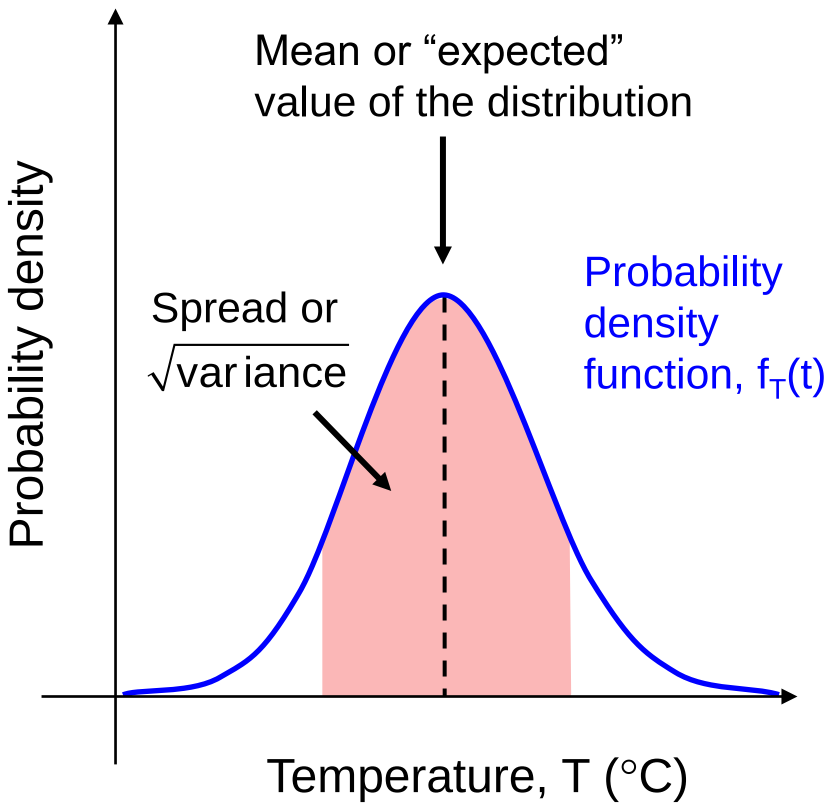


$$p = F_T(q)$$

$$q = F_T^{-1}(p)$$

Basic features

- The moments of a probability distribution describe its basic characteristics
- The first moment is the mean or "location", also known as the expected value of T, E[T]
- The central moments subtract the mean, as location does not matter for higher moments
- The second (central) moment is the variance or "average uncertainty", third is skew, etc.



$$\text{mean} = E[T]$$
$$\text{variance} = E[(T - E[T])^2]$$
$$\text{skew} = E[(T - E[T])^3]$$

Independence and dependence

Definition of statistical independence

- Random variables may be “statistically independent”
- Value of one variable does not influence the other
- In other words: $f_{XY}(x,y)=f_X(x)f_Y(y)$ for all x and y
- Quite rare in hydrology, but we often assume it!

Types and measures of dependence

- Independence is well-defined. Dependence is tricky
- Different types of relationships and measures exist
- For example, linearly related variables are “correlated”

Advanced slides from Section 5

Recall this simple case

Output uncertainty defined analytically

- Linear model, g, uncorrelated inputs, X_i, output, Y

$$\mathrm{Var}(Y) = \sum_{i=1}^{m} \mathrm{Var}(X_i) \cdot \left(\frac{\partial g}{\partial X_i} \right)^2$$

- Output unc. = (sum of) input unc. * input sensitivity

Problems with this analytical approach

- Hydrologic models are nonlinear, i.e. g is nonlinear
- The inputs, X_i, are generally related (e.g. temp/prcp)
- Output, Y, rarely normal: mean/variance not enough

Importance of "large" sample size

How many samples is enough?

- The larger the sample, the closer the output to target
- But, computationally demanding for complex models!
- Variance of the output (Y) has a sampling error:

$$\mathrm{sd}(\hat{\sigma}_Y^2) \approx \sigma_Y^2 \sqrt{\frac{2}{n-1}}$$

Note: the sample standard deviation (sd) of the variance of Y increases with the variance of Y. Thus, outputs w/ large uncertainty need larger n!

- Inversely proportional to square root of sample size, n
- Sampling uncertainty declines only gradually with n
- Can improve this with "clever" sampling techniques

Answers to questions

Answers to questions

Q1. (B,C,D,F)

Q2. (A,B,C,E,F)

Q3. (C,D,E)

Q4. (A,E)

Q5. (B,C,E)

Q6. (A,C,E,F)

QA1. (A,E,F)