

# Designing a Cross-paradigm Modeling Framework

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- Engineer: a flowchart explicitly describing the elements of a system.
- Agent-based modeler (ABMer): a collection of agents and rules for their interaction.

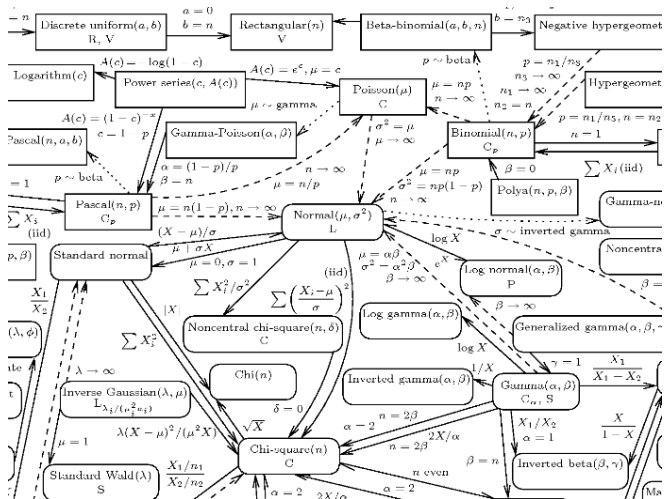
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- Engineer: a flowchart explicitly describing the elements of a system.
- Agent-based modeler (ABMer): a collection of agents and rules for their interaction.
- Empiricist: an observed distribution of occurrences.

# The Outline

- Motivation: why a standard model framework?
- Definition: Models as bundles of functions
- Some examples
- Filling in the blanks
  - ▶ Quick prototyping: you give me a likelihood function or an RNG; I'll test hypothesis about the model parameters.
- Transformation and combination operations
  - ▶ Both with pencil/paper and keyboard: a standard vocabulary for descriptive modeling
- A final example

# Transforming a model produces a new model



<http://www.math.wm.edu/~leemis/chart/UDR/UDR.html>

## Why do mathematicians formally define terms?

- If I use correctly-defined transformations on correctly defined atoms, I am guaranteed that the results are coherent.
- I can often determine what is *not* valid by inspection.
- Define transformations
  - ▶ Hierarchical models: the output from a set of child models feed data to a parent model.
  - ▶ Bayesian models: the output from a prior is used as a parameter set for the likelihood.
  - ▶ Structural equation models, causal models: simple models linked together to form a complex larger model.
- Modern computing technology
  - ▶ Formal definition maps immediately to structures and functions
- World peace
  - ▶ Monoids:  $[(\mathbb{N}, +), (\text{finite strings, concatenation}), (\text{models, cross})]$
  - ▶ There are commonalities across seemingly un-common genres.



## The computing slide

What structure is provided on top of FORTRAN '77?

- Some really are FORTRAN '77 with a pretty interface.
- Some provide tools for one genre only. [Can't use R for ABM; can't use Repast for regression.]
- Even some unifications are still only for small subsets of models: S's GLM model notation; King's Zelig, also for GLMs; BUGS/JAGS/R-BUGS for distributions + GLMs;
- Church, BLOG, Lisp-Stat: broad, unstructured frameworks

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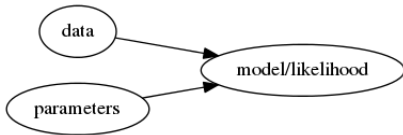
Apophenia, a C library

- This talk will not be an Apophenia tutorial or sales pitch. See <http://apophenia.info> .
- It will only have one slide with actual code.
- Please, implement this on your favorite platform, standalone or via front-end for Apophenia.

## Definition

# A model intermediates between data, parameters, and likelihoods

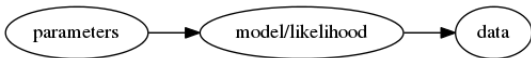
- data+parameters input: likelihood, or integrate to CDF



- data input: estimate parameters



- parameter input: draw random data, estimate most likely data



## Notation

- $\mathbb{D}$ : Data space. Anything required by the model; 'private' to the model unless otherwise noted.  $\leq$  is defined. [sample space]
- $\mathbb{P}$ : Parameter space. Similarly model-specific. [state space]
- $\mathbb{M}$ : Model space. The set of bundles of ML-consistent functions as per the next slide.

## A bundle of functions

A model is an internally consistent bundle of functions to intermediate between data, parameters, and likelihoods:

- Likelihood:  $(\mathbb{D}, \mathbb{P}) \rightarrow \mathbb{R}^+$ .
  - ▶ Integrates to a finite value; always nonnegative.
  - ▶ In some cases, better described as an 'objective function'.  
Doesn't have to integrate to one.
- Estimation:  $\mathbb{D} \rightarrow \mathbb{P}$ 
  - ▶ ML-consistency:  $L(\mathbf{d}, \mathbf{p})$  is maximized by  $\mathbf{p} = \text{EST}(\mathbf{d})$ .
- RNG:  $\mathbb{P}$  (and uniform prng)  $\rightarrow \mathbb{D}$ .
  - ▶ Likelihood of draw  $\mathbf{d} = \text{RNG}(\mathbf{p}) \propto L(\mathbf{d}, \mathbf{p})$ .
- CDF:  $(\mathbb{D}, \mathbb{P}) \rightarrow [0, 1]$ .
  - Proportion of random draws  $\text{RNG}(\mathbf{p}) \leq \mathbf{d} \rightarrow \text{CDF}(\mathbf{d}, \mathbf{p})$ .

## Alternatives to ML-consistency?

We could replace the consistency rule for  $\text{EST}$  using other consistency rules:

- KL-minimizing consistency
- Mean-squared-error minimizing
- Entropy-maximizing consistency
- Moments of  $\text{EST}(\mathbf{d})$  match moments of  $\mathbf{d}$ .

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But composing a entropy-maximizing model with a MoM model doesn't always make sense, so I stick to one genre here.



## Three examples

## The Normal example

- Likelihood:  $\mathcal{N}(x, \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-(x - \mu)^2/2\sigma^2)$  or  
 $\ln \mathcal{N}(x, \mu, \sigma^2) = -(x - \mu)^2/2\sigma^2 - \ln(2\pi\sigma^2)/2$ .
- Estimation:  $\hat{\mu} = \text{mean of } D$ ;  $\hat{\sigma} = \sqrt{\sum(d - \hat{\mu})^2/n}$ .
- RNG: See Devroye (1986).
- CDF: `gsl_cdf_gaussian_P(d-mu, sd)` (or see `erf`).

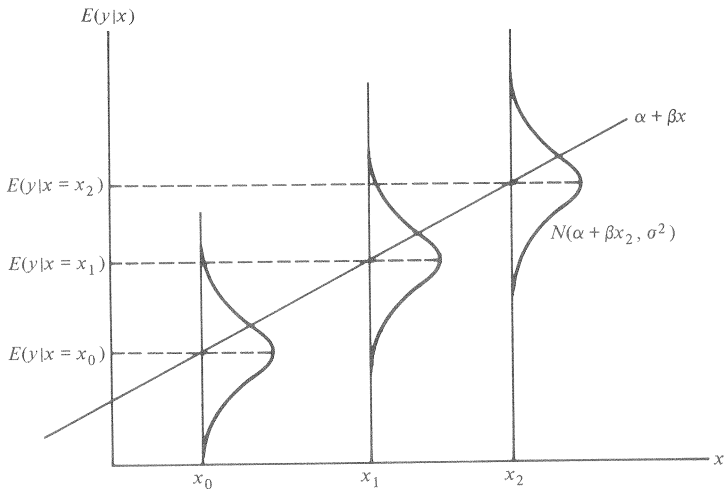
# The Discrete distribution (probability mass function, PMF)

A list of data items  $d_i$ ,  $i = 1 \dots N$ , with weights  $w_i$ .

- $\mathbb{D}$ :  $\mathbb{R}$ , categories, . . . .
- $\mathbb{P}$ :  $\{\emptyset, \mathbb{D}^1, \mathbb{D}^2, \dots, \mathbb{D}^N\}$
- Estimation: Copy input data  $\rightarrow$  parameters.
- Likelihood: If any elements in new data set  $\mathbf{x} \in \mathbb{D}$  are not  $\in d$ , zero. Else, product of matched weights.
- RNG: draw from  $d_i$ s weighted by weights.
- CDF: sort  $d_i$ s, sum weights.

# OLS

As given in the textbooks, not a consistent model by the defn here.



**FIGURE 5.3** The classical regression model.

[Greene, *Econometric Analysis*, 2<sup>nd</sup> ed., p 144]

# OLS

Undergrad stats consists of picking  $\mathbb{D}$ : should it be  
{BMI, age, sex, hours exercise/day},  
{BMI, age, sex, age $\times$ (is female), hours exercise/day},  
{BMI, age, sqrt(hours exercise/day)}, ... ?

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{BMI, age, sex, hours exercise/day},

{BMI, age, sex, age $\times$ (is female), hours exercise/day},

{BMI, age, sqrt(hours exercise/day)}, \dots ?

Given  $\mathbb{D}$ , starts as expected, but we hit a difficulty with RNG.

- $\mathbb{D}$ : as above,  $K$  variables.
- $\mathbb{P}$ :  $\beta \in \mathbb{R}^K$
- Estimation:  $\beta = (\mathbf{X}'\mathbf{X})^{-1}(\mathbf{X}'\mathbf{Y})$
- RNG: First, draw  $\mathbf{X}$  from a PMF built from the input data; then draw  $\epsilon$  from a  $\mathcal{N}(0, \sigma)$ ; then  $\mathbf{Y} = \mathbf{X}'\beta + \epsilon$ .
- Likelihood:  $(\mathbf{Y} - \beta\mathbf{X}) \sim \mathcal{N}(0, \sigma)$  (if  $\mathbf{X} \in \mathbf{D}$ ); see Normal model.

## With a standard interface, build standard procedures

- Testing: use the CDF or parameter models (and their CDFs).
- Bootstrapping, Jackknifing, Cook's distance: requires only estimation.
- MLE methods: as above, require only log likelihood; may use the score
- ML imputation: also requires only likelihood
- Tea: an R package for survey processing
- K-L divergence: use CDF or likelihoods; RNG can help if you want to do importance sampling

## A simulation example



## Just a likelihood

I only wrote down a likelihood function,  $P(\mathbf{D}, \mathbf{P})$ .

- Score (dlog likelihood): numeric deltas.
- Estimation: Use Maximum likelihood estimation.
  - ▶ All MLE algorithms repeatedly sample from the likelihood. Some use the score.
- RNG: ARMS (Gilks 1995)
- CDF: make random draws, count the percent up to a given point

## Just an RNG

I only wrote down a likelihood function,  $P(\mathbf{D}, \mathbf{P})$ .

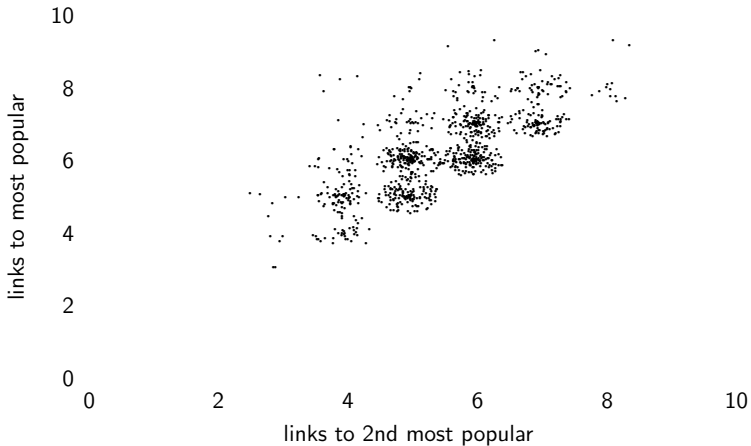
- Likelihood: make a million draws, write down a PMF using those draws.
- Estimation: give a likelihood, use prior slide.
- CDF: make random draws, count the percent up to a given point

## A network simulation (just an RNG)

Agents have randomly drawn individual positions, match based on proximity.

- Fix  $\sigma = 1$ .
- For each of  $N$  agents,
  - ▶ Draw  $N$  preferences  $(p_i)$  from a  $\mathcal{N}(0, \sigma)$ .
- For each pair of agents,
  - ▶ Link with probability  $1/(1 + |p_i - p_j|)$ .
- Count up links, report the sorted list of link counts for each agent.

## The two most popular outputs



**Figure:** A distribution of the number of links to the two highest-ranked members of a ten-person network (w/jitter).

## Our RNG defined a full model

We can calculate the other elements of the model from the RNG (memoize, use PMF).

- $H$ : the most popular agent has  $\leq 4$  links.
- $\text{CDF}_{NS}([4, 10, \dots, 10], \emptyset) \approx 0.0533$ .

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This was so easy to do, more people might start doing it.

Transforming models to produce other models:  $M \rightarrow M$

## The basic procedure

- Modify each element of the bundle
- Use defaults if needed
- Check the ML-consistency rules



## Fixed parameters

Start with a  $\mathcal{N}(\mu, \sigma)$ ; produce a  $\mathcal{N}(\mu, 1)$ .

- $\mathbb{D}$ : No change
- $\mathbb{P}$ : New space is reduced from original space
- Likelihood: Fix the parameter, use the base model's likelihood
- Estimation: MLE.
- RNG: Use the base model's.
- CDF: Use the base model's.

## More transformations

- Fixed parameters
- Constrained data
- Constrained parameters
- Jacobian transformations
- Smoothing (e.g., cubic splines, moving average)
- Kernel density (using another model as the kernel)

Joining models:  $(M, M) \rightarrow M$

## Stacking uncorrelated distributions

You need a Normal/Inverse Wishart prior for your Bayesian updating?

- $\mathbb{D}$ : Two options:  $\mathbb{D}_1 \times \mathbb{D}_2$  (if  $\mathbb{D}_1 = \mathbb{D}_2$ , one could send the same data to both models.)
- $\mathbb{P}$ :  $\mathbb{P}_1 \times \mathbb{P}_2$
- Likelihood:  $L_1(\mathbf{d}_1, \mathbf{p}_1) \cdot L_2(\mathbf{d}_2, \mathbf{p}_2)$
- Estimation: Independent estimations.
- RNG:  $(\text{RNG}_1(\mathbf{p}_1), \text{RNG}_2(\mathbf{p}_2))$
- CDF: use the default.

Easy to extend to three or more models.

## Output from model 1 $\Rightarrow$ input to model 2

- Four options:
  - ▶  $\mathbb{P}_{\text{out}} = \mathbb{D}_{\text{in}}$
  - ▶  $\mathbb{P}_{\text{out}} = \mathbb{P}_{\text{in}}$
  - ▶  $\mathbb{D}_{\text{out}} = \mathbb{D}_{\text{in}}$
  - ▶  $\mathbb{D}_{\text{out}} = \mathbb{P}_{\text{in}}$
- Aggregate model is a model in its own right, with its own  $\mathbb{P}$  and  $\mathbb{D}$  (but either may be  $\emptyset$ ).

## Parameter composition ( $\mathbb{D}_{\text{out}} = \mathbb{P}_{\text{in}}$ )

Instead of setting  $\mathbf{p}_2$  to a fixed value, draw  $\mathbf{p}_2$  from another distribution.

- $\text{RNG}_1 : \mathbb{P}_1 \rightarrow \mathbb{D}_1$
- $LL_2 : (\mathbb{D}_2, \mathbb{P}_2) \rightarrow \mathbb{R}$
- These are composable iff  $\mathbb{D}_1 \equiv \mathbb{P}_2$ . Then:
- $LL_2 : (\mathbb{D}_2, \text{RNG}_1(\mathbb{P}_1)) \rightarrow \mathbb{R}$

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We like to call  $M_1$  *the prior* and  $M_2$  *the likelihood*.

- If  $M_1$  and  $M_2$  are on the conjugate table, then the combination model is a closed-form distribution.
- Else, use Gibbs sampling to produce a PMF model.



## Data composition: multilevel modeling

- Do regressions for each classroom, producing params  $\beta^1, \dots, \beta^n$ .
- Then do a cluster analysis on the  $\beta$ s.
- I.e., use  $\mathbb{P}_{\text{out}}$  as  $\mathbb{D}_{\text{in}}$ .

## Data composition: evaluating the simulation

Continuing the example of the network model, which outputs a data set.

A link distribution has some well-known distributions: Zipf, exponential, . . . .

- $\text{RNG}_1 : \mathbb{P}_1 \rightarrow \mathbb{D}_1$
- $L_2 : (\mathbb{P}_2, \mathbb{D}_2) \rightarrow \mathbb{R}^+$
- Compose to produce  $L(\mathbf{p}_2, \text{RNG}_1(\mathbf{p}_1))$ .

Filling in the form:

- $\mathbb{D}$ :  $\emptyset$
- $\mathbb{P}$ :  $\lambda$
- Likelihood:  $L_2(\emptyset, \mathbf{p}_2)$
- Estimation: (Stochastic) MLE.
- RNG, CDF:  $\mathbb{D} = \emptyset$ .

## Data composition: use

- Above, we found the most likely  $\lambda$  from the simulation/evaluation model.
- Better: begin with a prior distribution on  $\lambda$  and use the sim/eval model to update to a posterior distribution on  $\lambda$ .

## OK, here's some code.

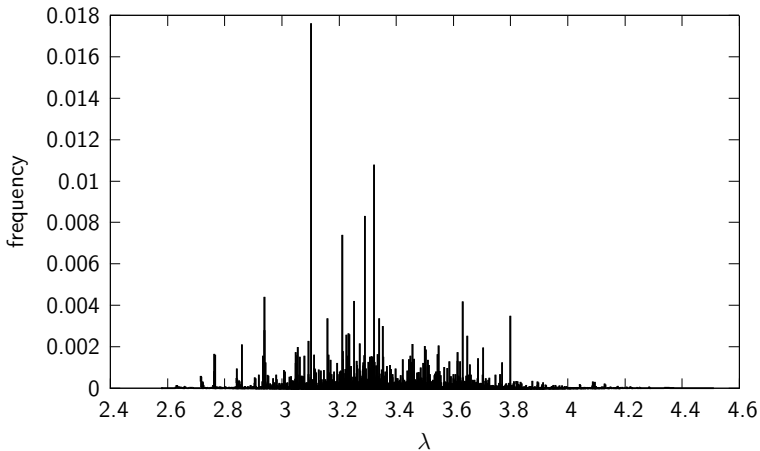
```
#include <apop.h>
#include "network_sim.c"

int main(){
    gsl_rng *r = apop_rng_alloc(1234);
    apop_model *comp = apop_model_dcompose(&network_sim,
                                           &apop_exponential, r);

    Apop_model_add_group(comp, apop_mle, .method=APOP_SIMAN);
    apop_model *estimated = apop_estimate(NULL, *comp);
    apop_model_print(estimated);

    apop_model *norm = apop_model_set_parameters(apop_normal, 3.5, .25);
    apop_model *post = apop_update(.prior=norm, .likelihood=comp);
    apop_data_pmf_compress(post->data);
    apop_data_sort(post->data);
    apop_model_print(post);
}
```

# Output



## A story problem

## The dinner party

- Two types come to my 8PM dinner party:
  - ▶ Tries to be on time, but hits a sequence of 10-minute delays, each with probability  $\lambda$ .
  - ▶ Shoots for 8:30, gets there on time  $\pm\epsilon$ .
- Nobody shows up early.

## The lateness model

$$M_{\text{mix}} = \text{mix}(\text{Jacobian}_{1/\lambda}(\text{Exponential}(\lambda)), \text{truncate}(\text{Normal}(\mu, \sigma)))$$

For the aggregate model:

- $\mathbb{P} = (\lambda, \mu, \sigma)$
- $\mathbb{D} = \mathbb{R}^+$  (arrival times)



## Don't forget priors

```
 $M_{\text{prior}} =$   
stack(  
  truncate(  
    Normal( $\mu_1, \sigma_1$ )  
  ),  
  Normal( $\mu_2, \sigma_2$ ),  
  Invert(  
    Wishart( $\Sigma$ )  
  )  
)
```

For  $M_{\text{prior}}$ :

- $\mathbb{P} = (\mu_1, \sigma_2, \mu_1, \sigma_2, \Sigma)$
- $\mathbb{D} = (\lambda, \mu, \sigma)$  (AKA  $\mathbb{P}_{\text{Mix}}$ )

# The whole thing

$$M_{\text{arrival}} = \text{DP-compose}(M_{\text{prior}}, M_{\text{mix}})$$

For  $M_{\text{arrival}}$ :

- $\mathbb{P}_{\text{arrival}} = (\mu_1, \sigma_1, \mu_2, \sigma_2, \Sigma)$
- $\mathbb{D} = \mathbb{R}^+$  (arrival times)

## The whole thing, written out

$$M_{\text{arrival}} = \text{DP-compose}(\text{stack}(\text{truncate}(\text{Normal}(\mu_1, \sigma_1)), \text{Normal}(\mu_2, \sigma_2), \text{Invert}(\text{Wishart}(\Sigma))), \text{mix}(\text{Jacobian}_{1/\lambda}(\text{Exponential}(\lambda)), \text{truncate}(\text{Normal}(\mu, \sigma)))$$

## Using the model

Reduced to a nonparametric PMF:

- Fix  $\mathbb{P}_{\text{arrival}}$  and find a posterior PMF of arrival times (Bayesian updating).
  - ▶ Then, do data-space evaluations, e.g. K-L divergence( $M_{\text{arrival}}$ , PMF (data)).

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As a parameterized model:

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## The conclusion slide

We can formally define a model as a bundle of functions that are internally consistent.

It's a simple definition, but it lets us:

- Apply standard tools to simulations, ML models, . . . .
- Implement complex models using simple components (both at the keyboard and AFK).
- Describe disparate statistical situations in a consistent manner.
  - ▶ Clarify inconsistencies and reveal new applications of old tools.
  - ▶ Try methods from different genres of modeling.