Geostatistical inference under preferential sampling: Final presentation

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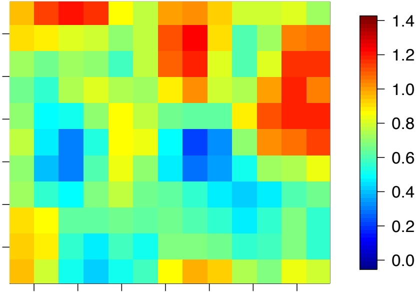
Divisions of Spatial Statistics

- Cressie (1991) and Gelfand (2010) divide spatial statistics into 3 areas:
  - discrete data
  - continuous data
  - point patterns



Data simulated with `RandomFields` R package (Schlather et al., 2016)

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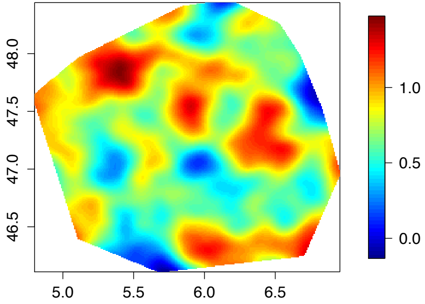

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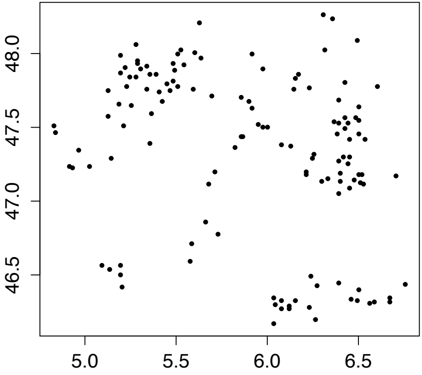

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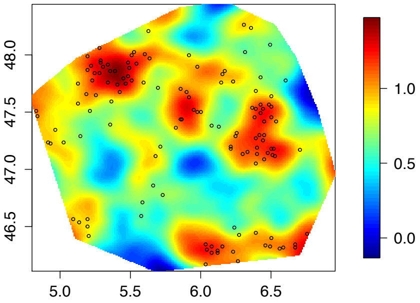
Divisions of Spatial Statistics

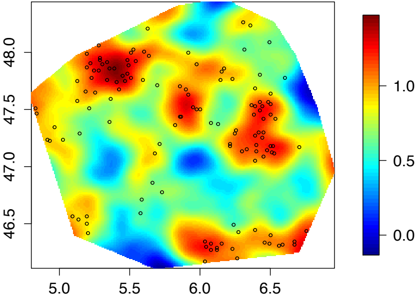
- Cressie (1991) and Gelfand (2010) divide spatial statistics into 3 areas:
  - discrete data
  - continuous data
  - point patterns
- Diggle et al. (2013) instead gives 2 subdivisions of spatial statistics:
  - continuous data
  - discrete data
- This emphasizes random nature of sampling locations



Data simulated with `RandomFields` R package (Schlather et al., 2016)

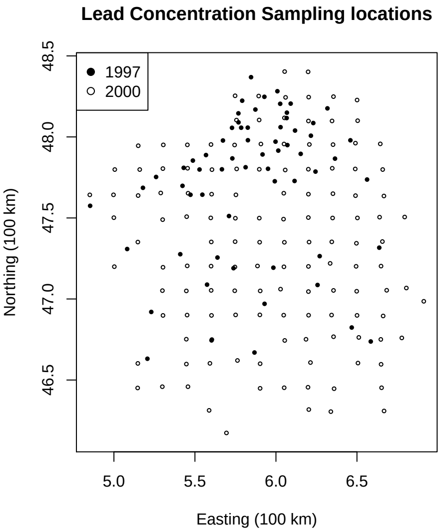
Divisions of Spatial Statistics

- Classically, data locations are assumed to be fixed constants
- What happens when the sample locations depend on the measured process itself?
  - This is called **preferential sampling**



Problems Addressed

- Determining if data is sampled preferentially
- How preferential sampling affects 'naive' inference
- Effective model for preferential sampling
- Focus on lead levels in Galicia, Spain and simulated experiments



Classical Model

$$Y_i = \mu + S(x_i) + Z_i,$$

Y_i: observation at location x_i

μ: mean

$S(\vec{x}) \sim \text{MVN}\left(\vec{0}, \Sigma(\vec{x})\right)$: spatially correlated portion of process

$Z_i \overset{iid}{\sim} \mathcal{N}\left(0, \tau^2\right)$: measurement noise

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Log likelihood:

$$\mathcal{L}(\vec{\theta}) = -\frac{1}{2}\log(|\Sigma_0|) - \frac{1}{2}(\vec{Y} - \vec{\mu})'\Sigma_0^{-1}(\vec{Y} - \vec{\mu}) - \frac{n}{2}\log(2\pi)$$

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Common assumptions:

- x_i are sampled independently of true process $\mu + S$
- Stationarity

Variograms

- **Stationarity**: under stationarity,
  $\text{Var}\left(S(x_i) - S(x_j)\right) = V(x_i - x_j)$
- **Isotropy**: under isotropy (and stationarity),
  $\text{Var}\left(S(x_i) - S(x_j)\right) = V(|x_i - x_j|)$
- **Variograms** define the spatial structure of the covariance in S
- Empirical estimate given data Y_i at location x_i (under stationarity and isotropy):

  $$\widehat{V}(d) = \frac{1}{|N(d)|} \sum_{|x_i - x_j| \in N(d)} (Y_i - Y_j)^2$$

  where $N(d)$ is the set of pairs (x_i, x_j) with $|x_i - x_j| \approx d$
- This estimator assumes non-preferentiality

Variograms

Matérn theoretical variogram:

$$V(d) = \sigma^2(1 - \rho(u \mid \phi, \kappa)) + \tau^2$$

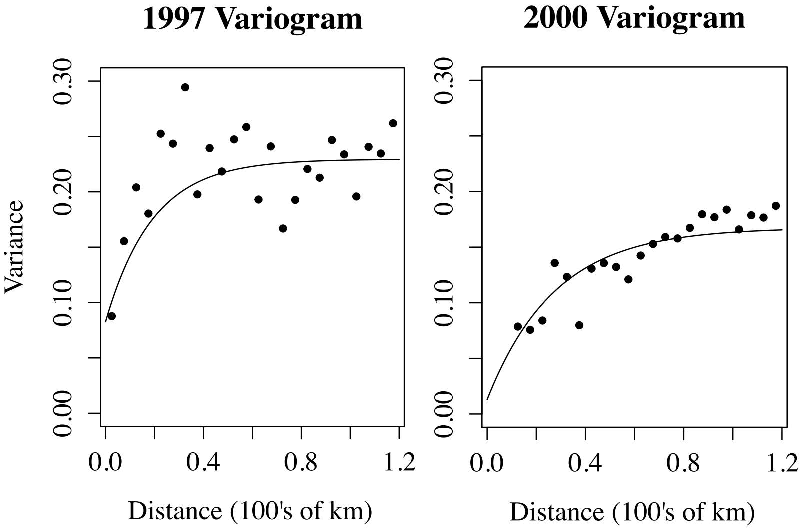
where

$$\rho(u \mid \phi, \kappa) = \frac{1}{2^{\kappa-1}\Gamma(\kappa)}(u/\phi)^\kappa K_\kappa(u/\phi),$$

is the Matérn correlation function

u: distance
ϕ: scale
κ: smoothness
σ^2: is the variance of S
τ^2: measurement variance
$K_\kappa(\cdot)$: Bessel function

Variograms of Log-Lead Data (Classical)



Model for Preferential Sampling

Three assumptions for model:

1. S is still a stationary, mean zero Gaussian process (so $S(\vec{x}) \sim \text{MVN}\left(\vec{0}, \Sigma(\vec{x})\right))$
2. Conditional on S, $\vec{X}$ is an inhomogeneous Poisson process wtih random intensity

$$\Lambda(x) = \exp\{\alpha + \beta S(x)\}$$

3. $Y_i | S, \vec{X} \overset{iid}{\sim} \mathcal{N}\left(\mu + S(x_i), \tau^2\right)$

$1 + 2 \Leftrightarrow X$ is a log Gaussian Cox process (LGCP)

Log-Gaussian Cox Processes

A **Cox process** is a stochastic point process that for B, B' bounded Borel sets satisfies:

- $\Lambda(x) \geq 0$ is a random intensity
- $N(B) \sim Pois\left(\int_B \Lambda(x)\, dx\right)$
- $N(B) \perp\!\!\!\perp N(B')$ when $B \cap B' = \emptyset$

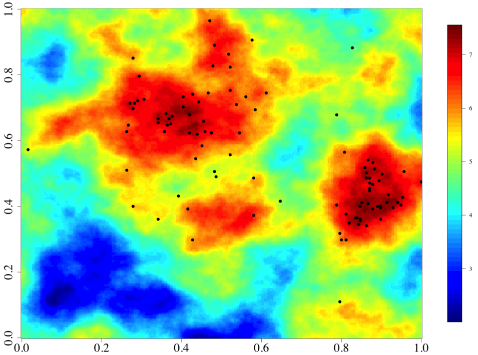
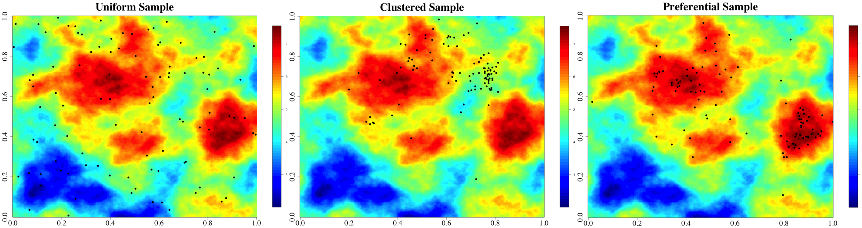


Figure: An example of a LGCP on unit square where $\beta = 2$, and S has Matérn covariance.

Testing Affect of Sample Designs: Samplings Schemes



Sampling processes for Matérn covariance, $\beta = 2$, and $\alpha = 1$.

Variogram estimation tested under 500 simulations from three sampling designs:

a Uniform

b Preferential ($\beta = 2$)

c Clustered

Classical Variogram Bias Under Preferential Sampling

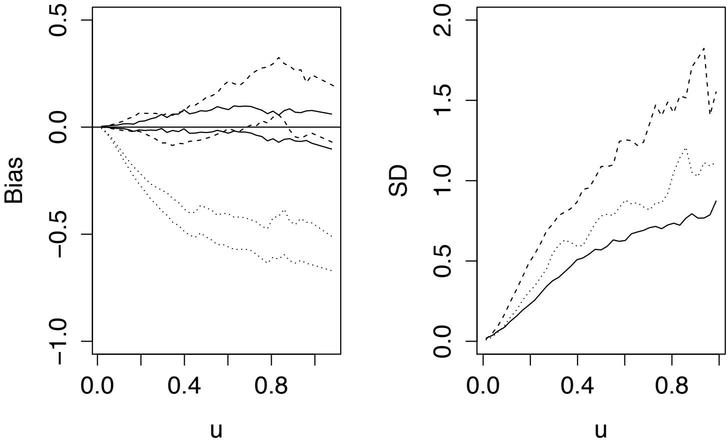


Figure: Variogram bias ± 2 standard errors and standard deviations for uniform (solid), clustered (dashed), and preferential (dotted) sampling schemes.

Classical Prediction Bias Under Preferential Sampling

Mod.	*Param.*	*Confidence intervals*		
		Uniform	*Preferential*	*Clustered*
1	Bias	(-0.03, 0.04)	(0.96, 1.13)	(-0.07, 0.06)
1	RMSE	(0.38, 0.42)	(1.31, 1.52)	(0.69, 0.79)
2	Bias	(-0.03, 0.02)	(-0.11, -0.06)	(-0.02, 0.04)
2	RMSE	(0.30, 0.32)	(0.32, 0.34)	(0.30, 0.32)

Table: Classical predictions using 95% Confidence intervals for the given parameters under the given models and sampling schemes

Models:

1. $(\mu = 4, \sigma^2 = 1.5, \phi = .15, \kappa = 1, \beta = 2)$
2. $(\mu = 1.51, \sigma^2 = .14, \phi = .31, \kappa = .5, \beta = -2.20, \tau^2 = .059)$

Preferential Model Likelihood

Make gridded approximation of $\vec{S} = \{\vec{S}_0, \vec{S}_1\}$ on lattice $\vec{X}^* = (x_1^* \ldots x_N^*)'$.

- $\vec{S}_0$ are true values at data locations
- $\vec{S}_1$ are true values at other grid points

$$
\begin{aligned}
L(\vec{\theta}) &= \int \pi(\vec{Y}|\vec{X}, \vec{S})\pi(\vec{X}|\vec{S})\pi(\vec{S})\ d\vec{S} \\
&= \ldots \\
&= E_{\vec{S}|\vec{Y}}\left[\pi(\vec{X}|\vec{S})\frac{\pi(\vec{Y}|\vec{S}_0)}{\pi(\vec{S}_0|\vec{Y})}\pi(\vec{S}_0)\right] \\
&\approx m^{-1}\sum_{j=1}^{m}\pi(\vec{X}|\vec{S}_j)\frac{\pi(\vec{Y}|\vec{S}_{0j})}{\pi(\vec{S}_{0j}|\vec{Y})}\pi(\vec{S}_{0j})
\end{aligned}
$$

where $\vec{S}_j$ is the jth conditional simulation of S conditioned on $\vec{Y}$.

Preferential Model Likelihood

Define C as a $n \times N$ matrix with a single 1 in each row and all else 0 s.t. $\vec{X} = C\vec{X}^*$.

Steps for Monte Carlo Simulation:

1. Simulate $\vec{S} \sim \text{MVN}\left(\vec{0}, \Sigma\right)$ using Circulant Embedding (Wood and Chan, 1994)
2. Compute jth simulation of $\vec{S}|\vec{Y}$:

$$\vec{S}_j \equiv \vec{S} + \Sigma C' \Sigma_0^{-1}(\vec{Y} - \vec{\mu} + \vec{Z} - C\vec{S})$$

   Where $Z_i \overset{iid}{\sim} \mathcal{N}\left(0, \tau^2\right)$

3. Calculate $m^{-1} \sum_{j=1}^{m} \pi(\vec{X}|\vec{S}_j) \frac{\pi(\vec{Y}|\vec{S}_{0j})}{\pi(\vec{S}_{0j}|\vec{Y})} \pi(\vec{S}_{0j})$

Preferential Model Likelihood

$$\pi(\vec{X}|\vec{S}_j) = \left(\prod_{i=1}^{n} \Lambda(x_i)\right)\left(\int \Lambda(x)\ dx\right)^{-n}$$

$$\vec{Y}|\vec{S}_{0j} \sim \mathrm{MVN}\left(\vec{S}_{0j}, \tau^2 I\right)$$

$$\vec{S}_{0j}|\vec{Y} \sim \mathrm{MVN}\left(\Sigma C'\Sigma_0^{-1}(\vec{Y} - \vec{\mu}), \Sigma - \Sigma C'\Sigma_0^{-1} C\Sigma\right)$$

$$\vec{S}_{0j} \sim \mathrm{MVN}\left(\vec{0}, C\Sigma C'\right)$$

Goodness of Fit

Reduced second moment measure (or K-function) for defined model is given by:

$$K(s) = \pi s^2 + 2\pi \int_0^s (\exp\left\{\beta^2\sigma^2\rho(u;\kappa,\phi)\right\} - 1)u \; du$$

s: distance
$\rho(u;\phi,\kappa)$: Matérn correlation function

K-functions commonly used in goodness of fit tests

Goodness of Fit: Monte Carlo Testing

For any Monte Carlo test statistic, T, where higher T casts doubt on H_0, assume:

- T_1 is from data
- $T_2, ..., T_n$ are simulated under H_0

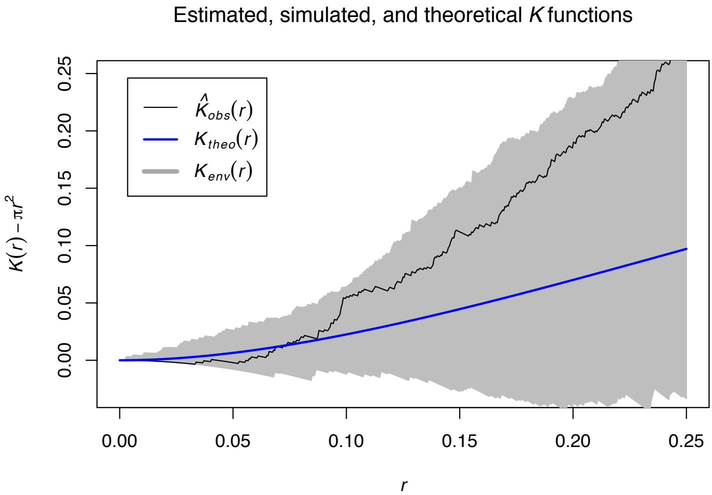
Then our p-value is the rank of T_1 out of $T_1, T_2, ..., T_n$ (*i.e.* if $n = 100$ and T_1 is largest test statistic, $p = .01$).

Goodness of Fit: Test Statistic

$$T = \int_0^{0.25} \frac{\left(\hat{K}(s) - K(s)\right)^2}{v(s)}\, ds$$

$K(s)$: Theoretical K-function under MLEs
$\hat{K}(s)$: Empirical K-function of simulation (or data)
$v(s)$: Variance of $\hat{K}(s)$

Goodness of Fit: Monte Carlo Testing



$p = 0.07$

Likelihood Fitting

- Use Nelder-Mead (Nelder and Mead, 1965) simplex algorithm for optimization with naive initial guesses
  - To simulate the $\vec{S}_j$'s quickly, I use cutoff embedding (Gneiting et al., 2012)
- Standard errors and correlations for MLEs inferred using quadratic fit of likelihood surface

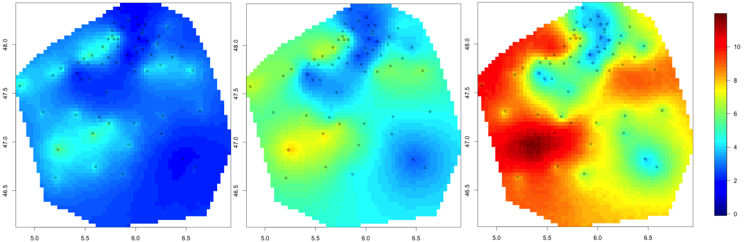
Likelihood Fit: Non-Preferential

	Estimate	*SE*	*Correlation matrix*				
μ_{97}	1.55	0.018	1	0.00	0.02	-0.00	-0.02
μ_{00}	0.73	0.014		1	0.10	0.20	0.07
σ	0.37	0.006			1	0.39	-0.37
ϕ	0.31	0.039				1	0.47
τ	0.23	0.005					1

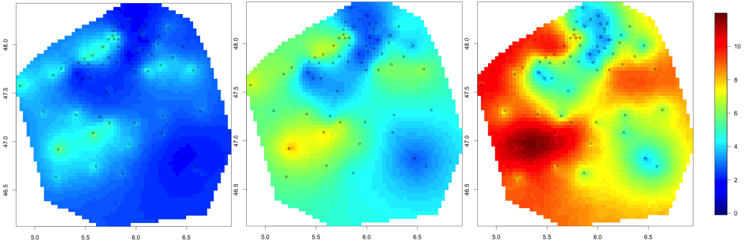
Table: Estimates are under joint 1997 and 2000 model

- Likelihood ratio test performed for joint versus separate models:
  - $p = 0.007$ under 3 degrees of freedom

1997 Predictions



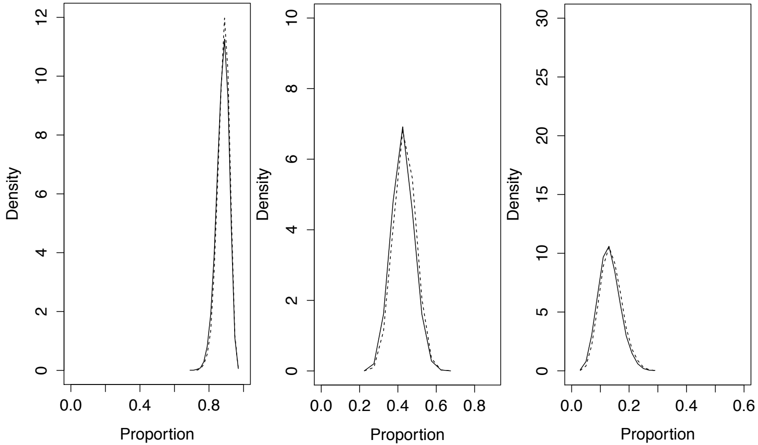
Preferential (MLEs from (Diggle et al., 2010)): ($\hat{\mu}_{97} = 1.515$, $\hat{\mu}_{00} = 0.762$, $\hat{\sigma}^2 = 0.138$, $\hat{\phi} = 0.313$, $\hat{\tau}^2 = 0.059$)



Non-preferential (MLEs fit with naive initial guess):

($\hat{\mu}_{97} = 1.551$, $\hat{\mu}_{00} = 0.727$, $\hat{\sigma}^2 = 0.136$, $\hat{\phi} = 0.305$, $\hat{\tau}^2 = 0.052$)

1997 Predictions



Areal proportion predicted over 3 (left), 5 (middle) and 7 (right) μ g/(g dry weight) for preferential (solid) and non-preferential (dashed) MLEs

Problems with the Methodology

- Using the joint model for 1997 predictions
- Assuming independence of 1997 and 2000 data in fitting
- No cross-validation performed
- No evaluation of preferential model in simulation study
- True preferential predictive distribution not used nor given
  - True predictive distribution may be Gaussian, although its parameters are unclear
- Non-preferential MLEs similar to preferential MLEs:
  - My non-preferential model: $(\hat{\mu}_{97} = 1.551, \hat{\mu}_{00} = 0.727, \hat{\sigma}^2 = 0.136, \hat{\phi} = 0.305, \hat{\tau}^2 = 0.052)$
  - Their preferential model: $(\hat{\mu}_{97} = 1.515, \hat{\mu}_{00} = 0.762, \hat{\sigma}^2 = 0.138, \hat{\phi} = 0.313, \hat{\tau}^2 = 0.059)$

Conclusions

- Accounting for preferentiality is important
- For empirical variogram estimation and classical prediction:
  - Uniform sampling performed best, then clustered, then preferential
  - For preferential data, naive variogram estimates and predictions were biased
- Proposed class of models is flexible and tractable for geostatistics with preferential data

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Appendix: Understanding the Preferential Likelihood

$$
\begin{aligned}
L(\theta) &= \int_S [\vec{X}|\vec{S}][\vec{Y}|\vec{S},\vec{X}]\frac{[\vec{S}|\vec{X},\vec{Y}]_{np}}{[\vec{S}|\vec{X},\vec{Y}]_{np}}[\vec{S}]\ d\vec{S} \\
&= \int_S [\vec{X}|\vec{S}][\vec{Y}|\vec{S},\vec{X}]\frac{[\vec{S}|\vec{X},\vec{Y}]_{np}}{[\vec{S}_1|\vec{S}_0,\vec{X},\vec{Y}]_{np}[\vec{S}_0|\vec{X},\vec{Y}]_{np}}[\vec{S}_1|\vec{S}_0][\vec{S}_0]\ d\vec{S} \\
&= \int_S [\vec{X}|\vec{S}]\frac{[\vec{Y}|\vec{S},\vec{X}]}{[\vec{S}_1|\vec{S}_0,\vec{X},\vec{Y}]_{np}[\vec{S}_0|\vec{X},\vec{Y}]_{np}}[\vec{S}_1|\vec{S}_0][\vec{S}_0][\vec{S}|\vec{X},\vec{Y}]_{np}\ d\vec{S} \\
&= \int_S [\vec{X}|\vec{S}]\frac{[\vec{Y}|\vec{S}_0,\vec{X}]}{[\vec{S}_1|\vec{S}_0,\vec{X}]_{np}[\vec{S}_0|\vec{X},\vec{Y}]_{np}}[\vec{S}_1|\vec{S}_0][\vec{S}_0][\vec{S}|\vec{X},\vec{Y}]_{np}\ d\vec{S} \\
&= \int_S [\vec{X}|\vec{S}]\frac{[\vec{Y}|\vec{S}_0,\vec{X}]}{[\vec{S}_1|\vec{S}_0,\vec{X}]_{np}[\vec{S}_0|\vec{X},\vec{Y}]_{np}}[\vec{S}_1|\vec{S}_0][\vec{S}_0][\vec{S}|\vec{X},\vec{Y}]_{np}\ d\vec{S} \\
&= E_{[S|\vec{X},\vec{Y}]_{np}}\left[[\vec{X}|\vec{S}]\frac{[\vec{Y}|\vec{S}_0,\vec{X}]}{[\vec{S}_0|\vec{X},\vec{Y}]_{np}}[\vec{S}_0]\right]
\end{aligned}
$$