Hierarchical Bayesian spatial modelling with Multivariate, Nonstationary and Nonseparable processes for air pollution in Euskadi

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The spatial model

My way to deal with large geostatistical data

My way to deal with dense goestatistical data

Air contamination in Euskadi

What is at stake?

- Public health problem.
  - Surges in emergency admissions in hospitals after contamination peaks.
  - Long-term exposure even when there is no peak.
- Subsequent social justice problem due to environmental inequalities.
- Public policies assessment (low-emission zones, low-speed zones, wood-fired power plants).

Who are our culprits?

- Nitrogen Oxides (NO, NO_2, NO_X).
- Ozone.
- Fine particles of size 10 and $2.5\mu m$.

What is the format of our data?

- Fixed measurement stations.
- One observation per day.
- Some NAs.
- Some misalignment.

Modelling choices 1/2: the big decisions

We pursue a Bayesian **space-time** hierarchical model aiming to **interpolate** the data.

- No modelling of the diffusion and transformation processes.
- We can nonetheless assess the effect of some predictors using linear effects.

We want a **multivariate** model.

- "Borrow strength" between variables to have better predictions.
- Explore the correlations between those variables.

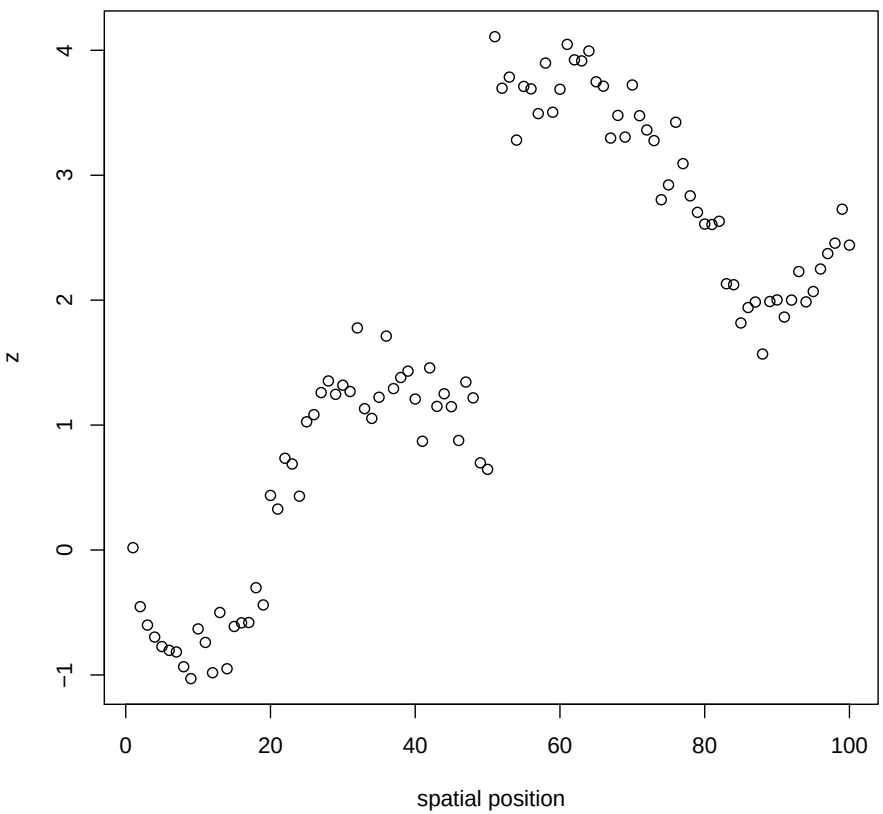
We want to separate long-term and short-term components.

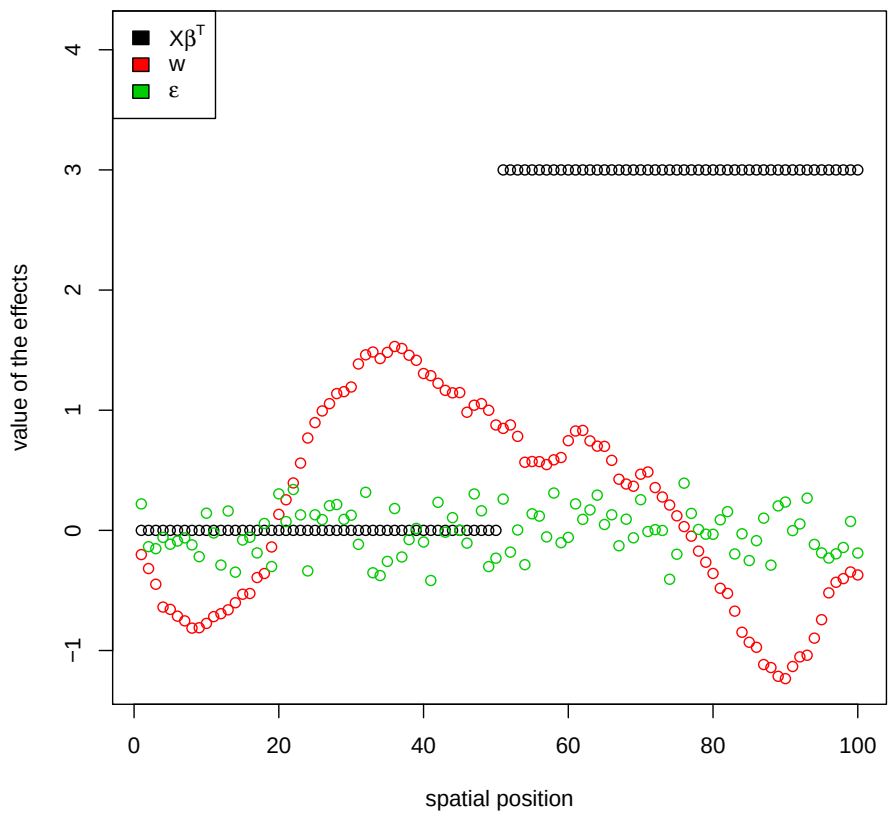
- Long-term exposure.
- Peaks.

Gaussian data model

The data is modelled using:

- Linear effects (like in a good old linear model).
- Noise (like in a good old linear model).
- A **spatially coherent** component not explained by the linear effects.





Example

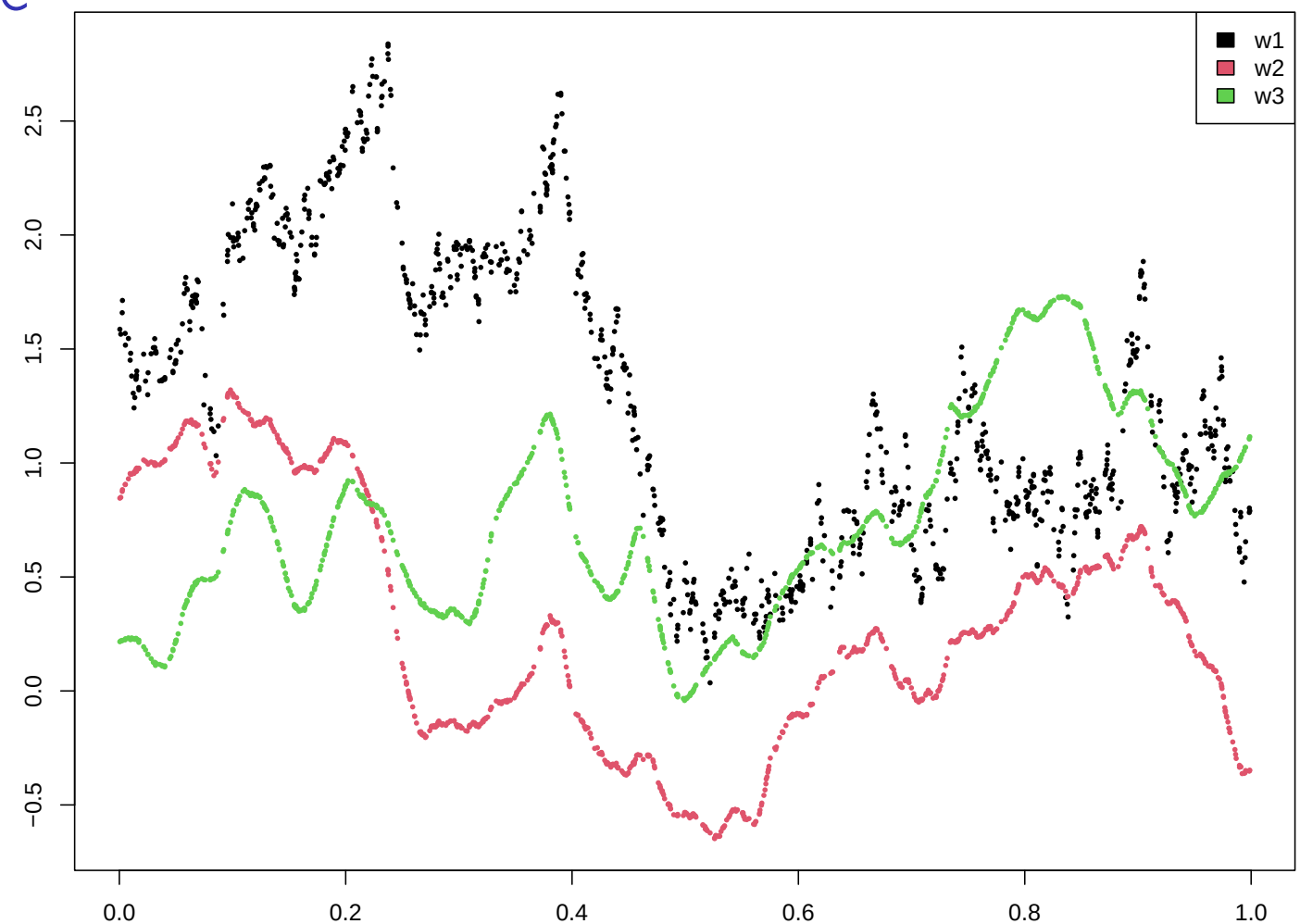
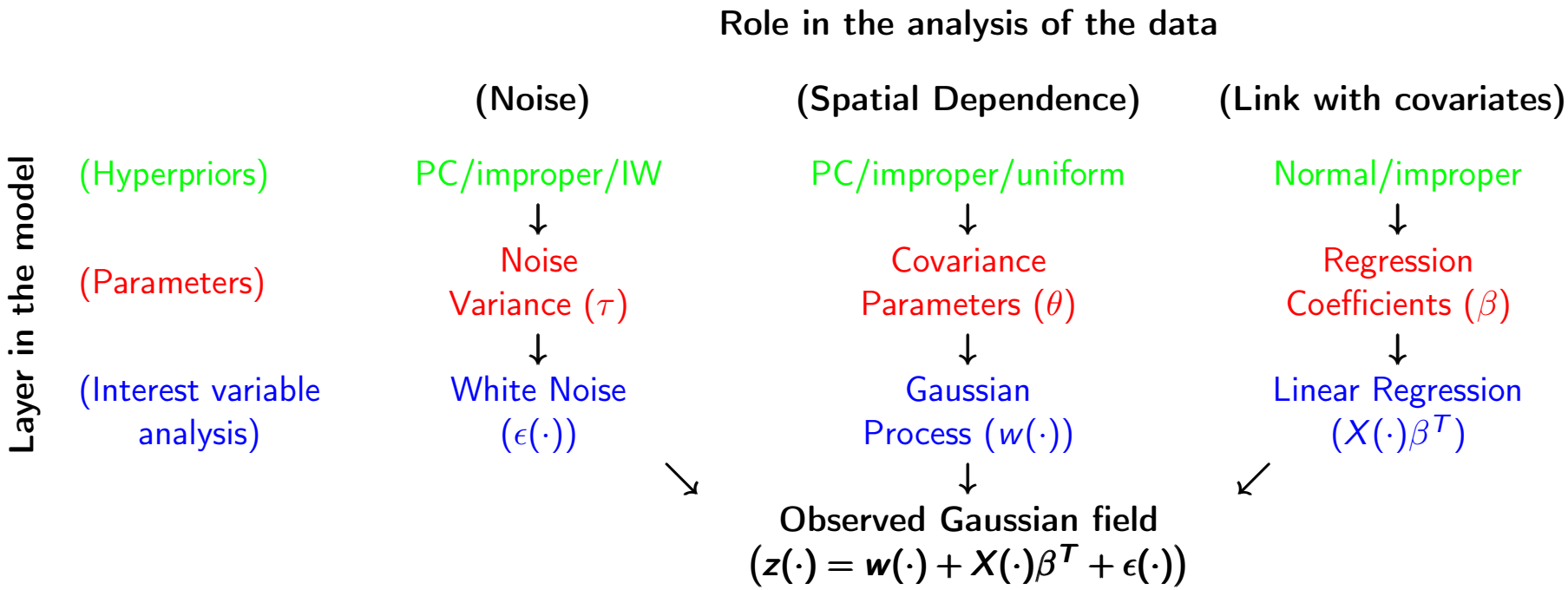


Figure 2: A multivariate Gaussian field

Hierarchical Model Architecture

The decomposition of the data is embedded in a **hierarchical model**:

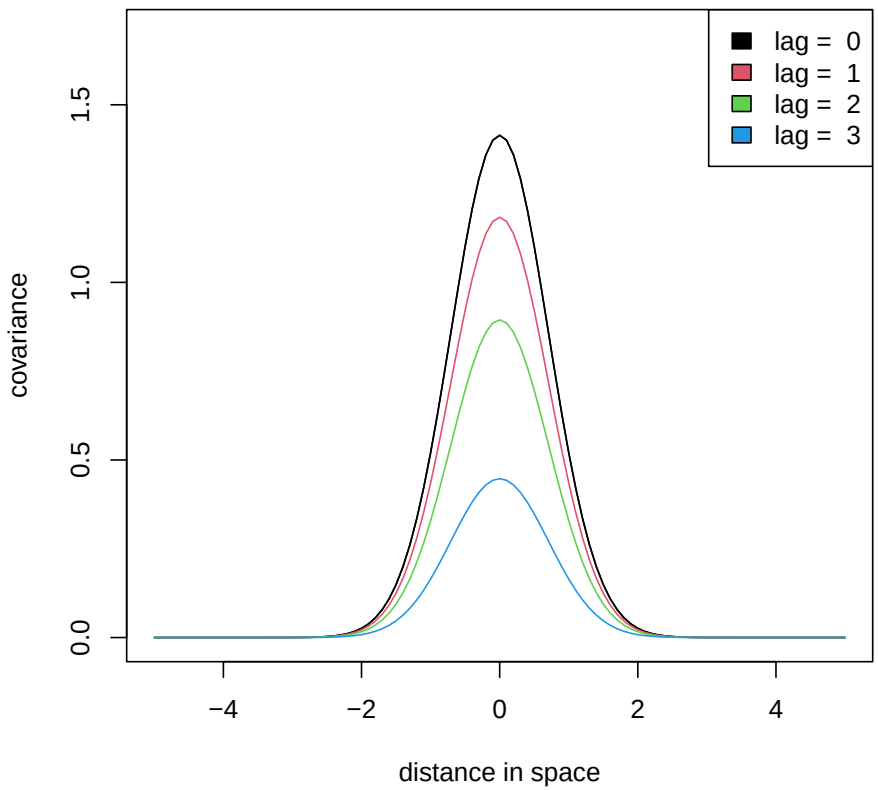
$$p(parameters, process|data) \propto$$
$$p(data|parameters, process)p(process|parameters)p(parameters).$$

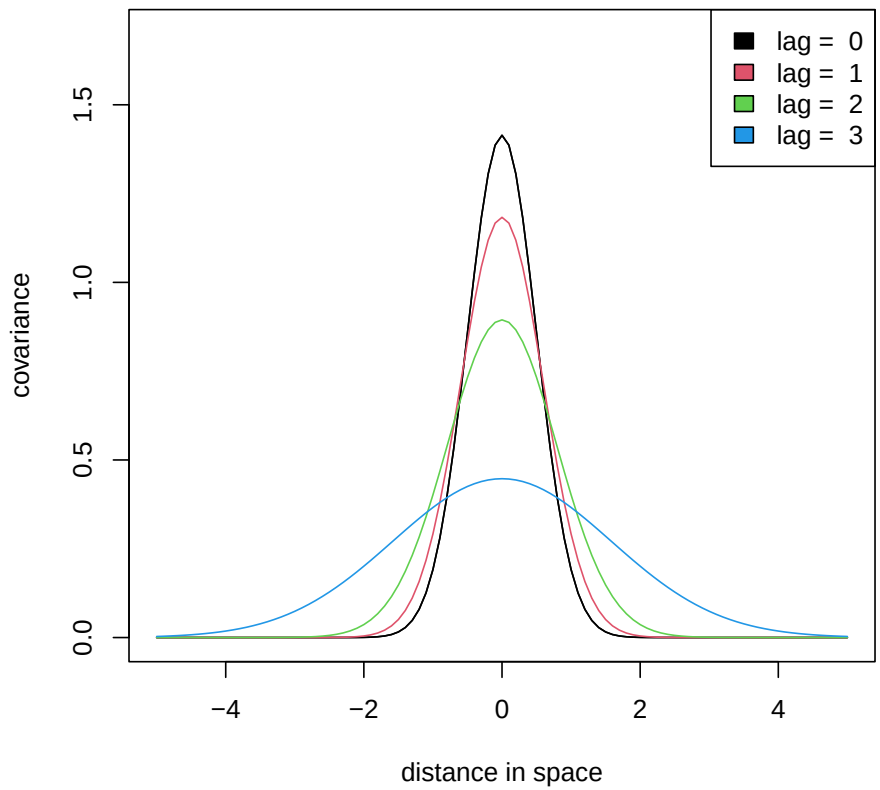


Nonseparability

I want to add **Nonseparability**, using the work of Allard et al. (2022).

- Better performance in prediction Allard et al. (2022).
- Better interpretation of the diffusion of a pollutant.





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Un problème de taille [1]

The **marginal dimensions** of the data set are **misleading**. In a data set with...

- $n_{var} = 4$ variables (that's Iris).
- $n_{space} = 10000$ spatial sites (with Inla you need 10 minutes).
- $n_{time} = 3500$ measurements in time (10 years of daily measurements - just perfect to teach time series to your students).

... we get **140 M** observations. And that is not all!
We need to set up a **denser** model, with:

- Space links because we have a spatial component.
- Time links because we have a temporal component.
- Space-time links because of nonseparability.
- Links between several variables to evaluate multivariate correlations.

[1] In French: "a matter of size" / "a big problem"

Objectives for the implementation

I would like to have an **efficient** and **scalable** implementation.

- Something that can be run from a laptop for a "moderate" ($10^5 - 10^6$ observations) data set.
- Something that can exploit the capacities of a cluster.

In practice, what does it take?

- Control CPU use.
- Control RAM use.
- Allow for **parallelization**.
  - Introduce parallelizability...
  - and avoid **bottlenecks**!
- Use GPUs?

Nearest Neighbor Gaussian Process approximation

Problem: allow the covariance parameters to dictate the behavior of the latent field. The naive case (kriging) is

- $O(n^3)$ FLOPs.
- $O(n^2)$ RAM.

We need to use an approximation that is

- cheap in RAM.
- cheap in FLOPs.
- parallelizable.

A Nearest Neighbor Gaussian Process approximation looks like an **Auto-Regressive model** (for time series) but with a **spatial component**.

- Linear FLOP and RAM cost in the number of observations.
- Embarrassingly parallelizable.
- Induces **sparsity**.

But is that enough when you have millions of observations?

Recursive Nearest Neighbor Gaussian Processes

Idea: compute the approximation **for only 1 time period** and recycle it!
Restrictions:

- The measurements must be **regularly spaced in time**.
- The measurement sites must be **fixed in space**.
- The process must be **stationary in correlation** (nonstationary marginal variance is still allowed).

Strengths:

- No need for full observations (NAs are perfectly OK).
- No need to have all the variables observed at a measure site (I can have only NOX and Ozone in one site, PMs in another site, etc).
- **The cost does not depend on the number of time periods!**

Parallel programming in R

How to do parallel computing in R?

- With parallel or its loop-friendly version foreach.
- With omp through Rcpp.
- With future.

Problems:

- in Windows, parallel needs to **copy** the objects it uses.
- parallel does not allow to modify objects from each thread, you need to **collect** and **re-process** the results.
- omp **crashes when you put some R** in the loop.
- with parallel, there is an **overhead** depending empirically on:
  - a **fixed cost**.
  - the **RAM size** of the **outputs**.
  - the **RAM size** of the **inputs**.

My approach:

- use a **stepwise approach**.
- things that should work well do not always work well.
- the reverse is much less frequent.

Cutting corners (of the matrix)

The upper corner of the covariance patrix between a point and its parents is **block-Toeplitz** with **symmetric blocks**.

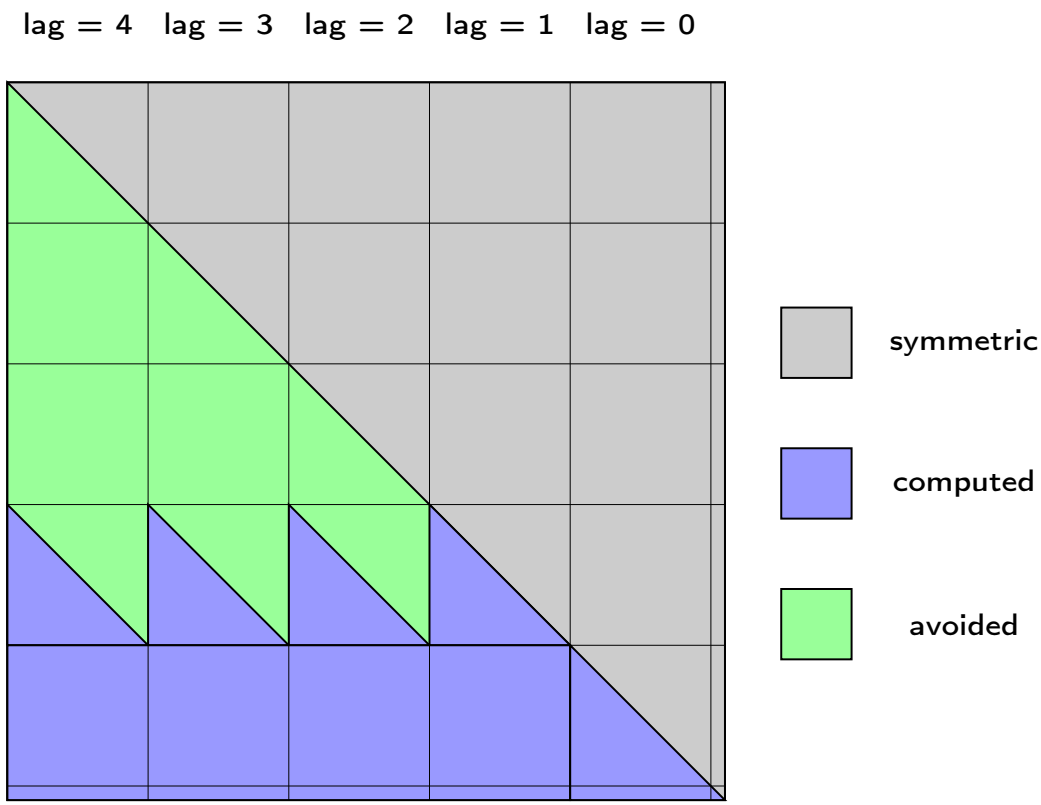

Figure 4: Avoided computations in the covariance matrix

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Updating the latent field

The latent field has two problems:

- space-time autocorrelation.
- coupling with the high-level parameters.

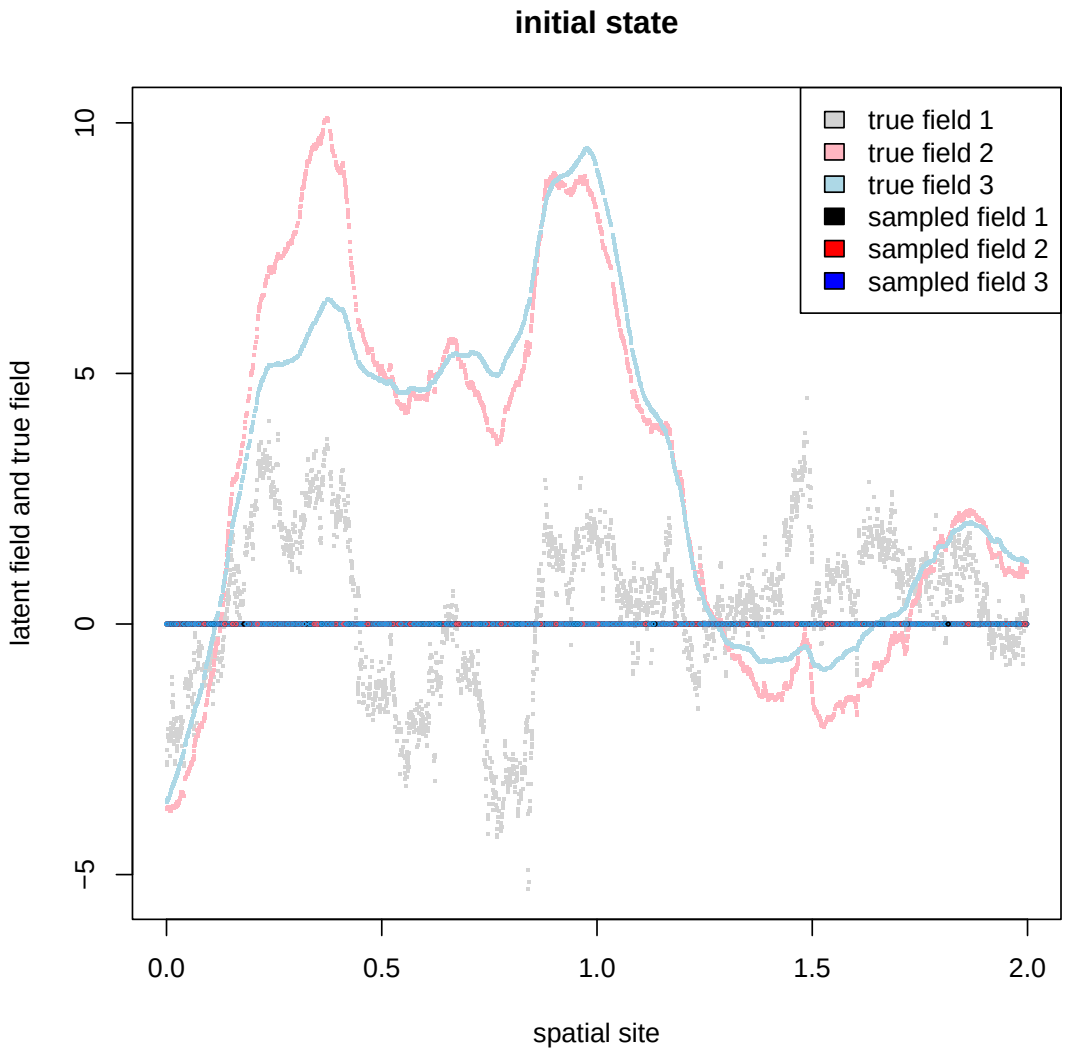
Those two problems need **sampling from the latent field** to be solved.

- The update groups must be **small** to limit the cost of an update.
- The clusters must be **large** to deal with spatial auto-correlation.

Original solution: using a **blocks-and-bases** sampling with **spatially coherent perturbations**.

- Parallelizable thanks to chromatic schemes like in Coube-Sisqueille and Liquet (2021).
- Deals with auto-correlation thanks to various resolutions.
- Cheap thanks to sparsity of the basis functions (tapering).

Only blocks (usual algorithm)



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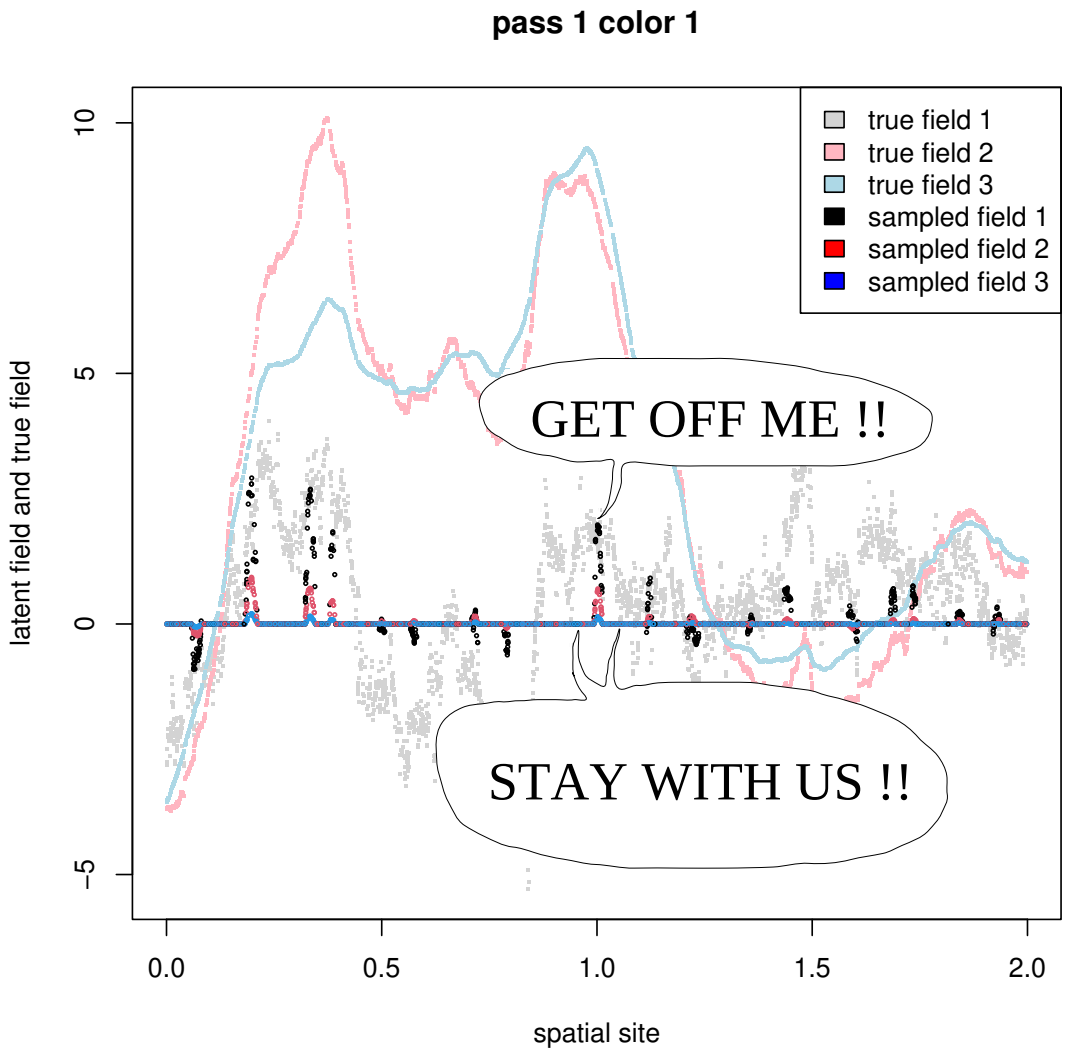

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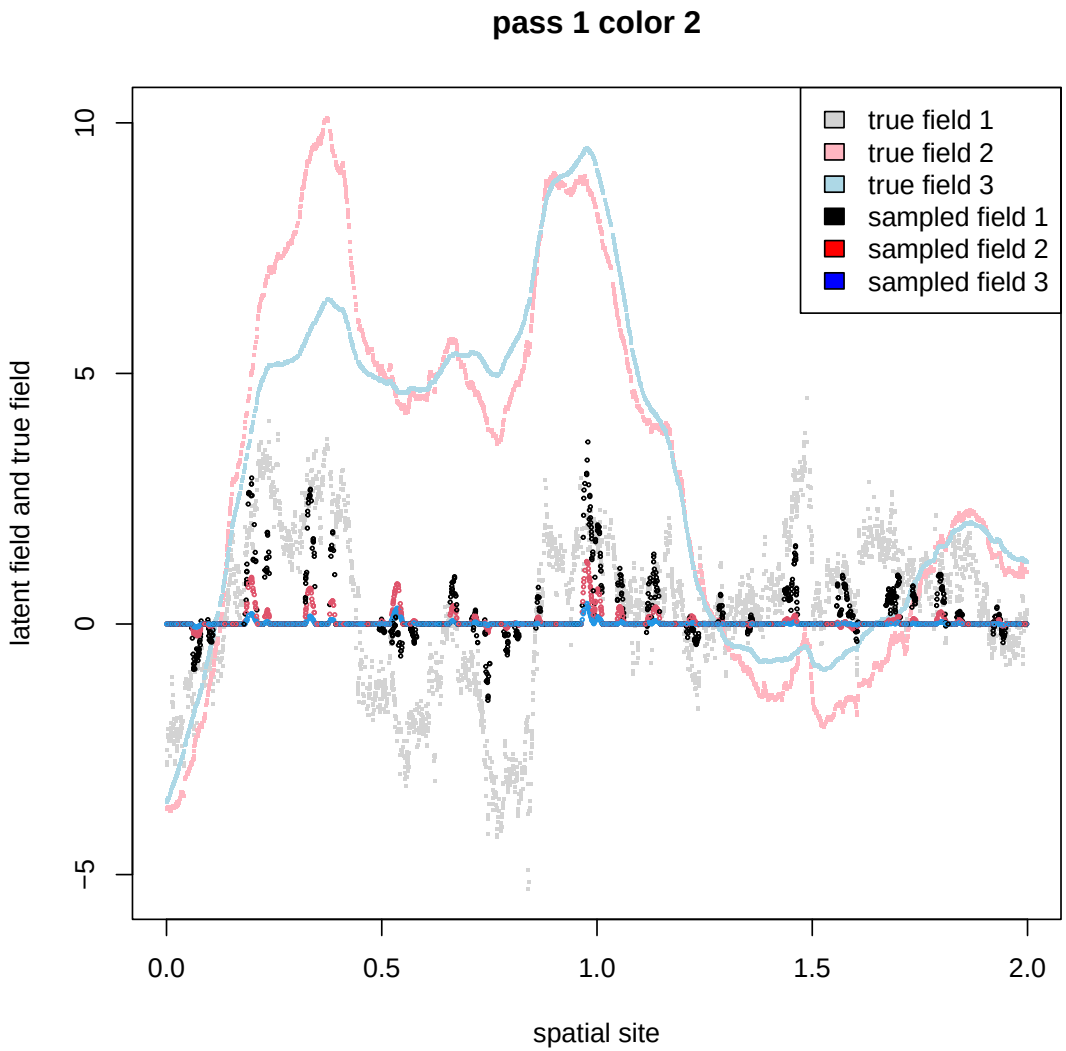

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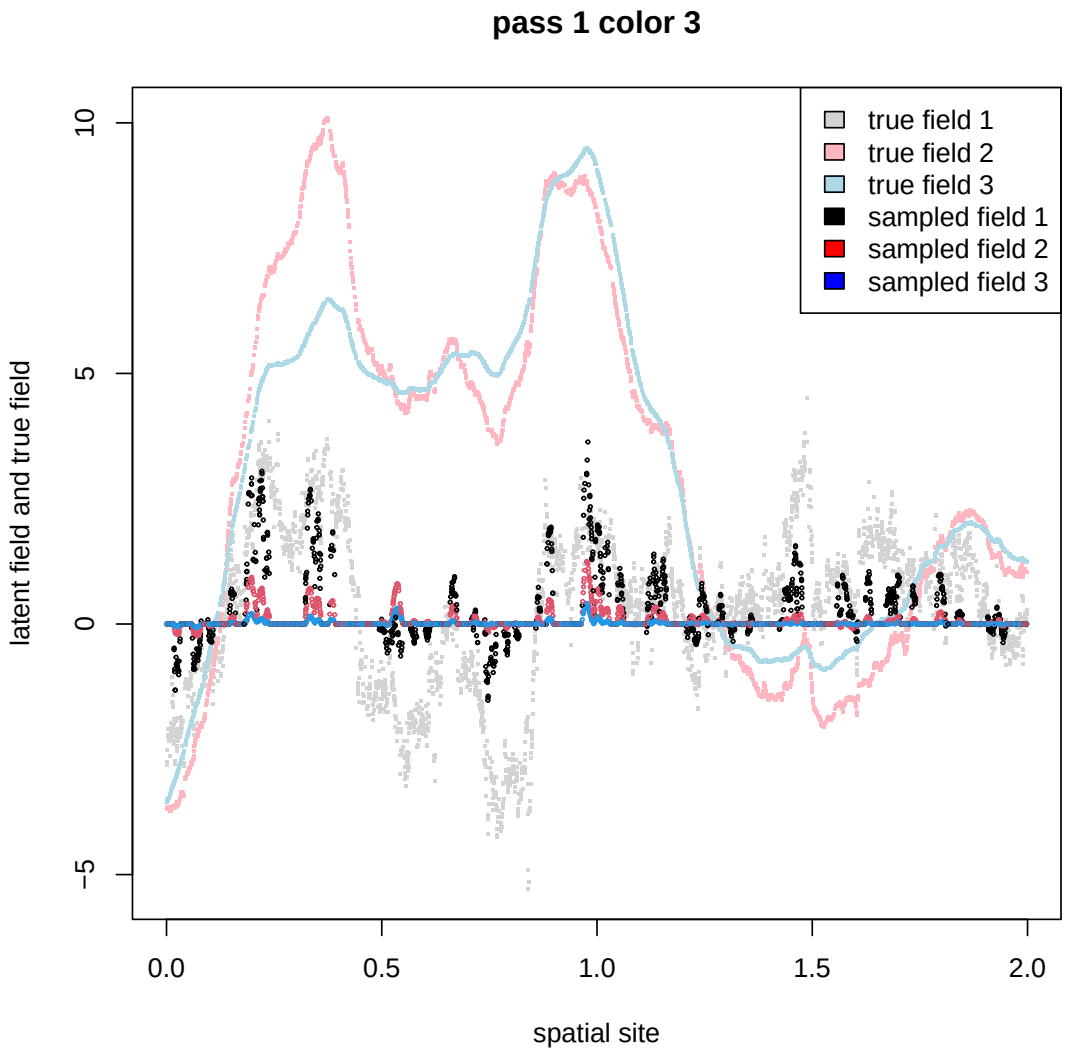

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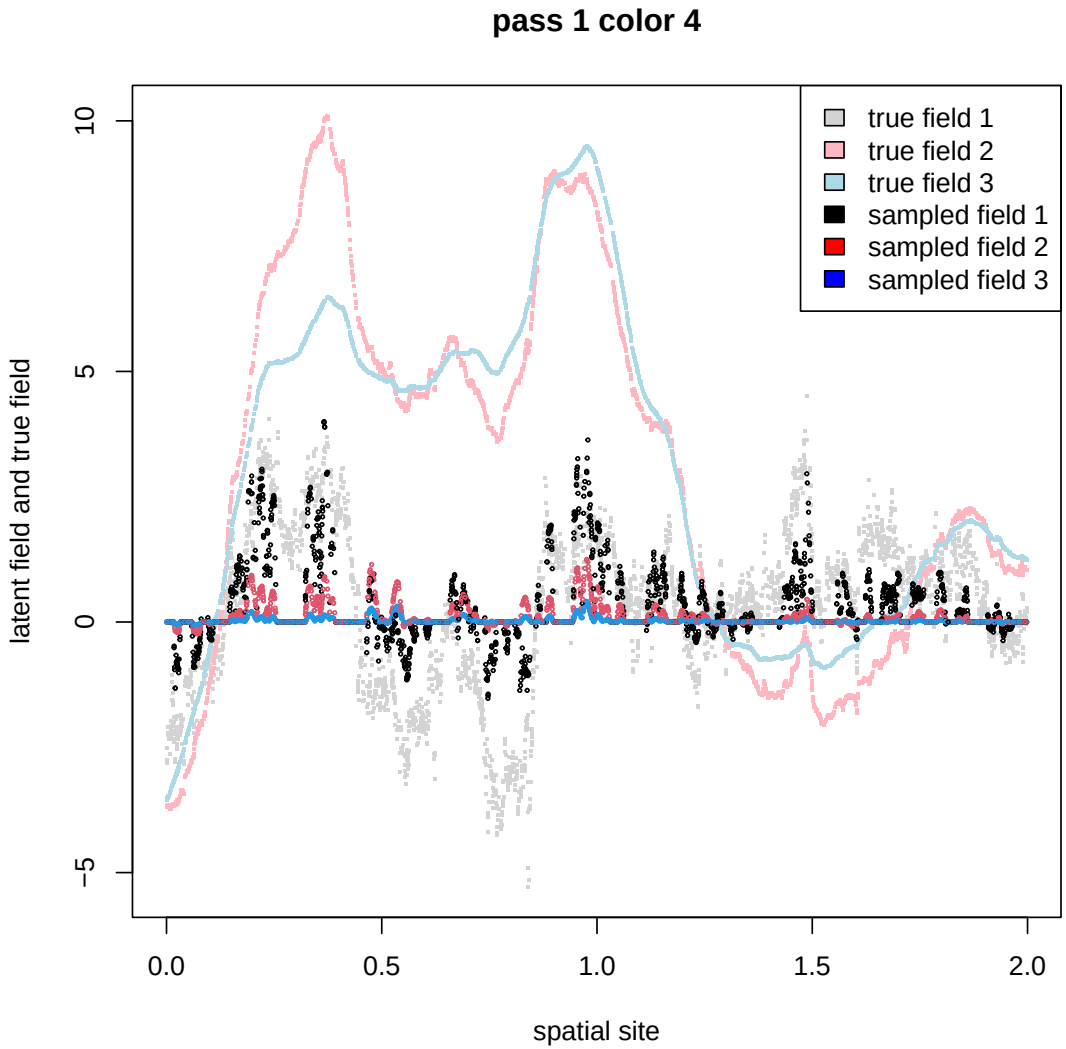

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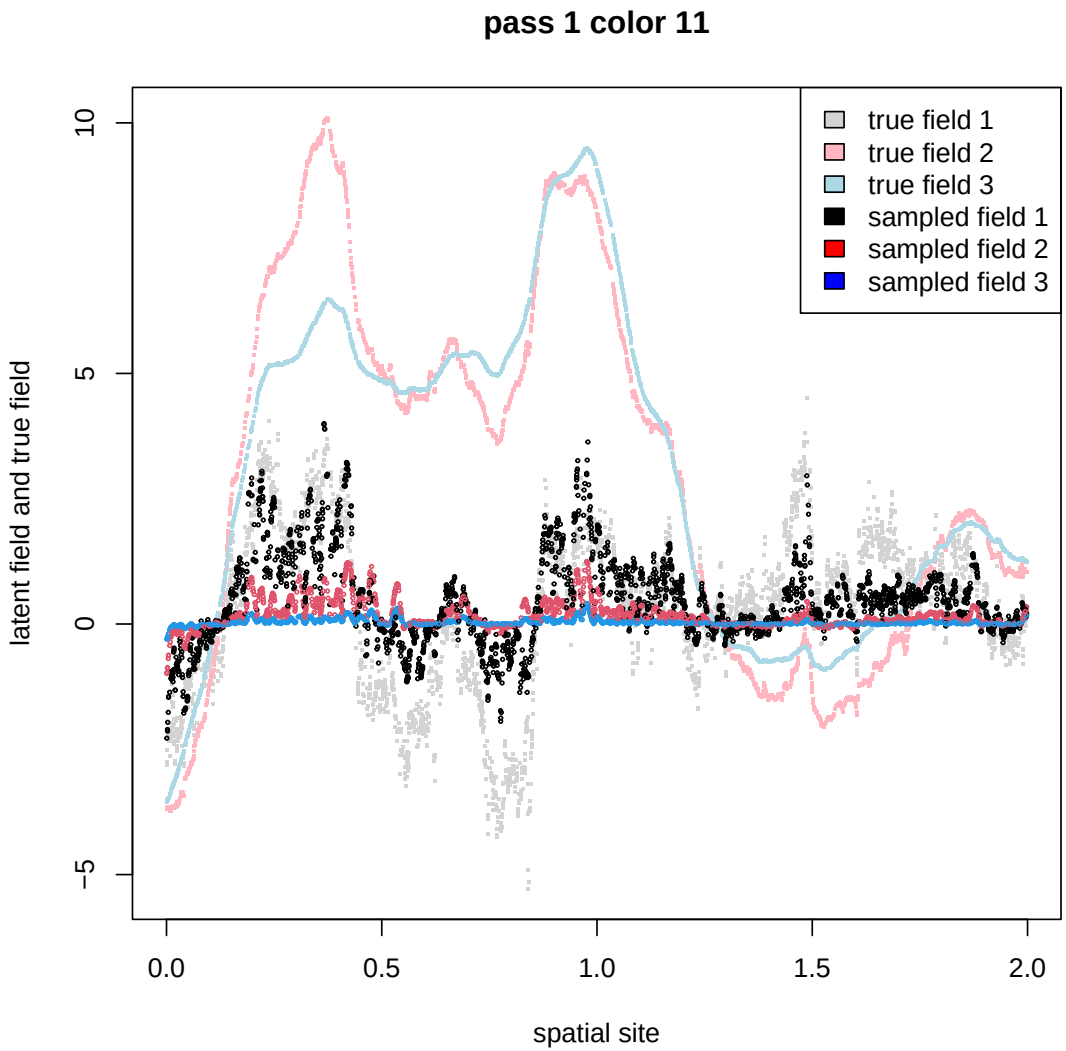

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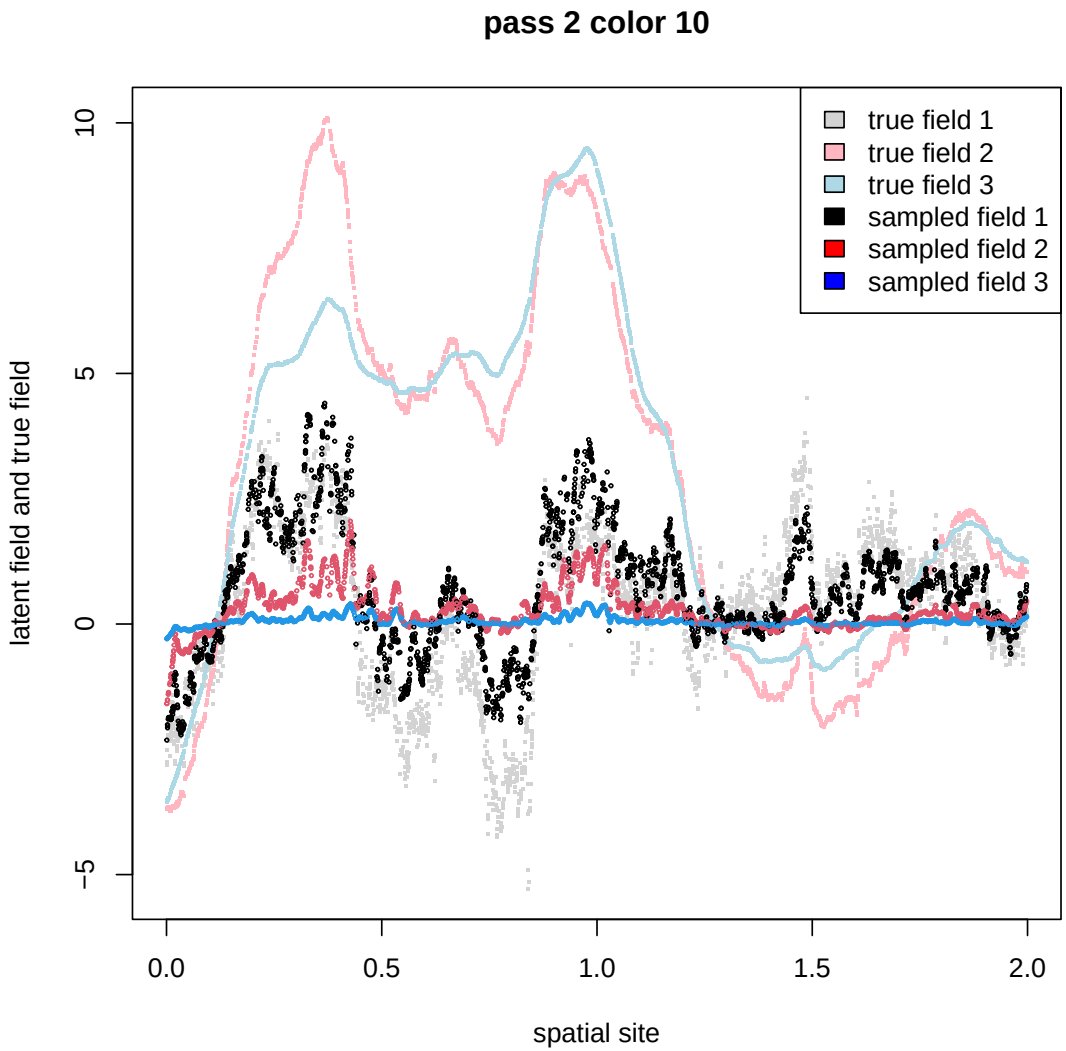

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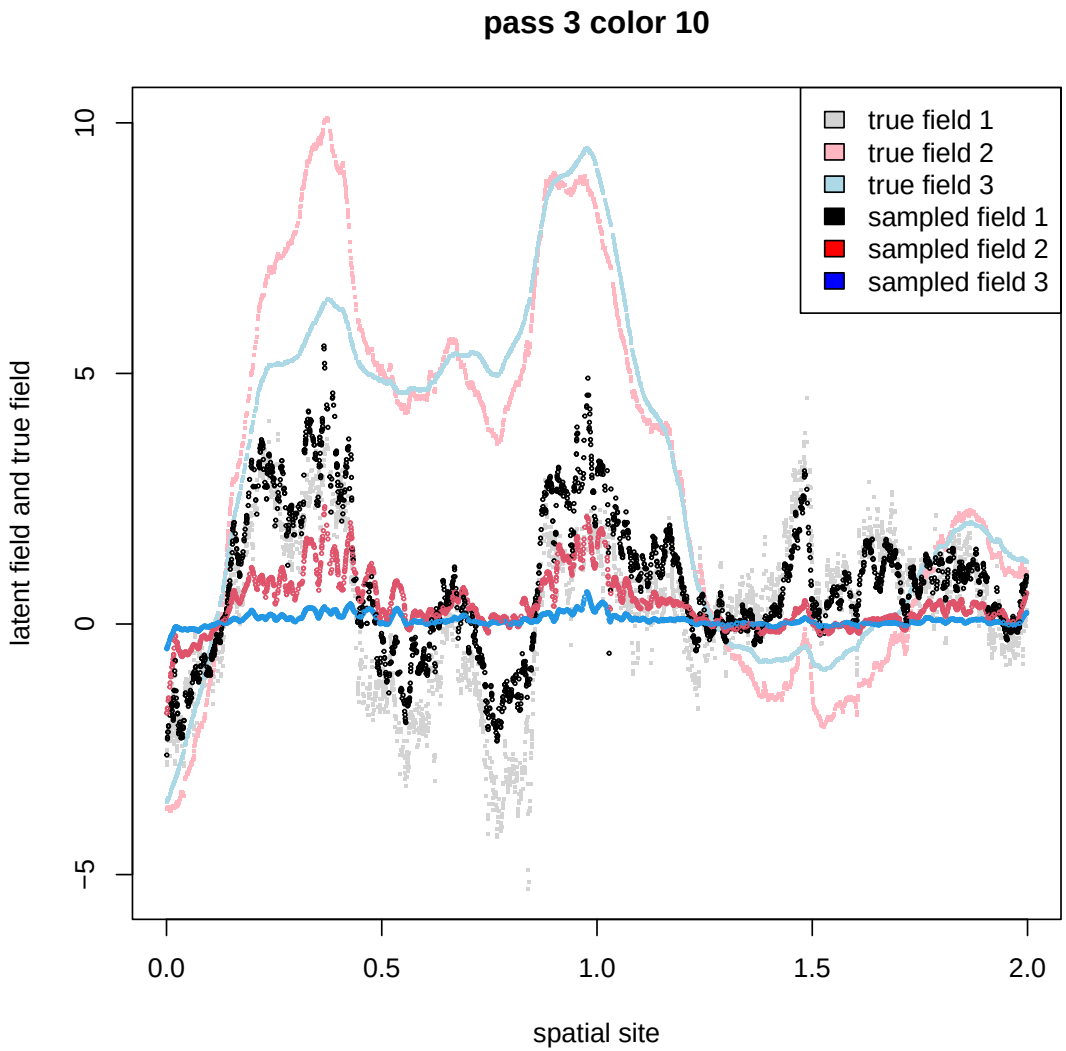
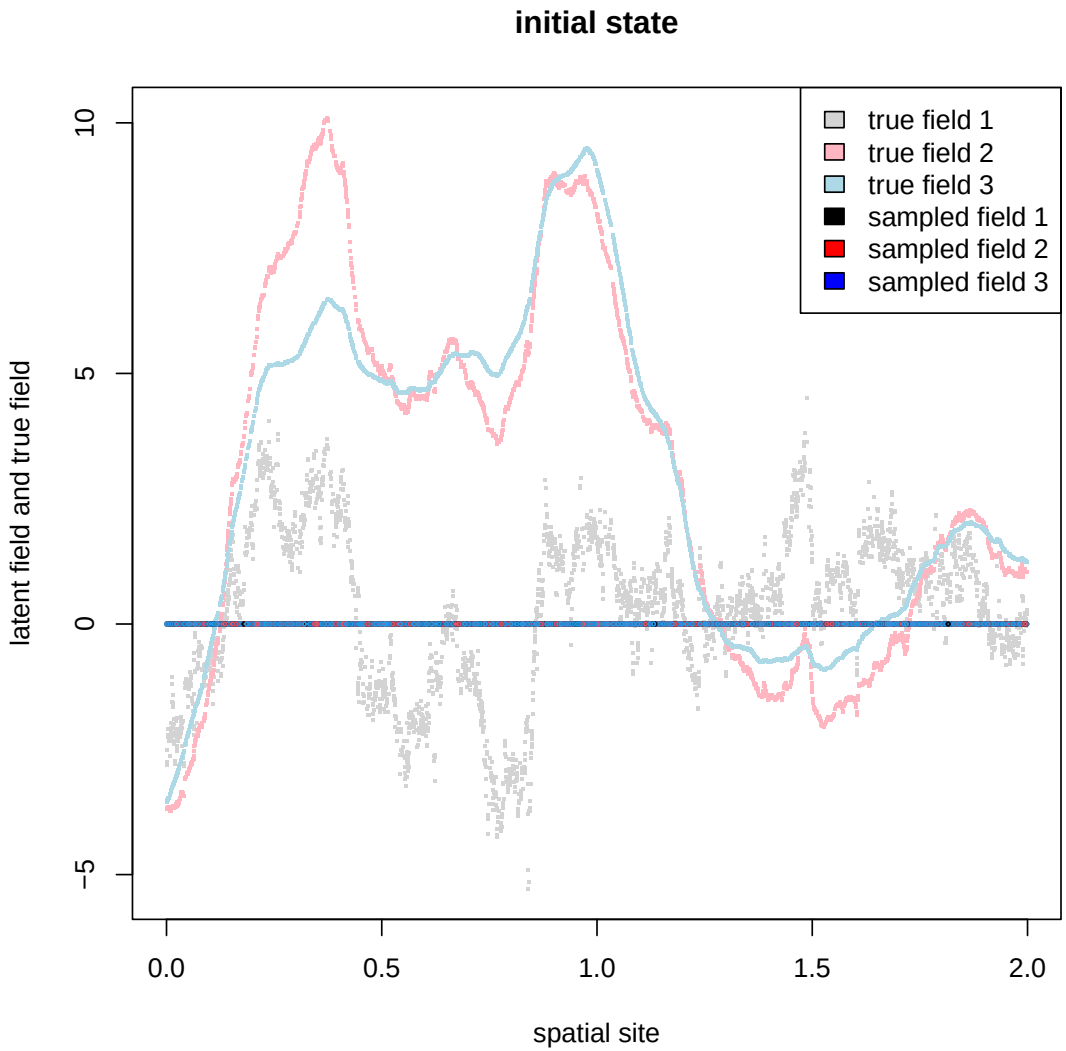


Blocks 'n' Bases



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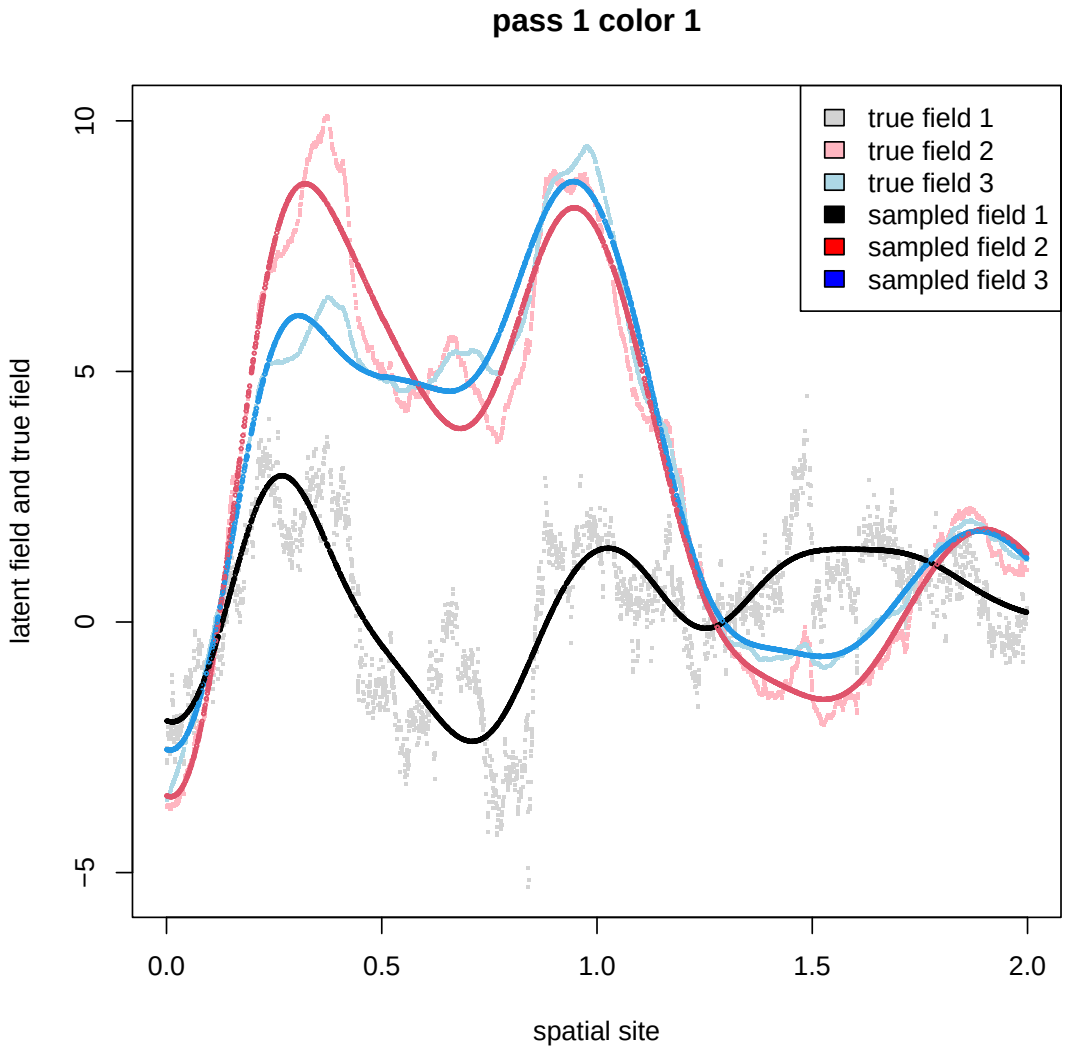

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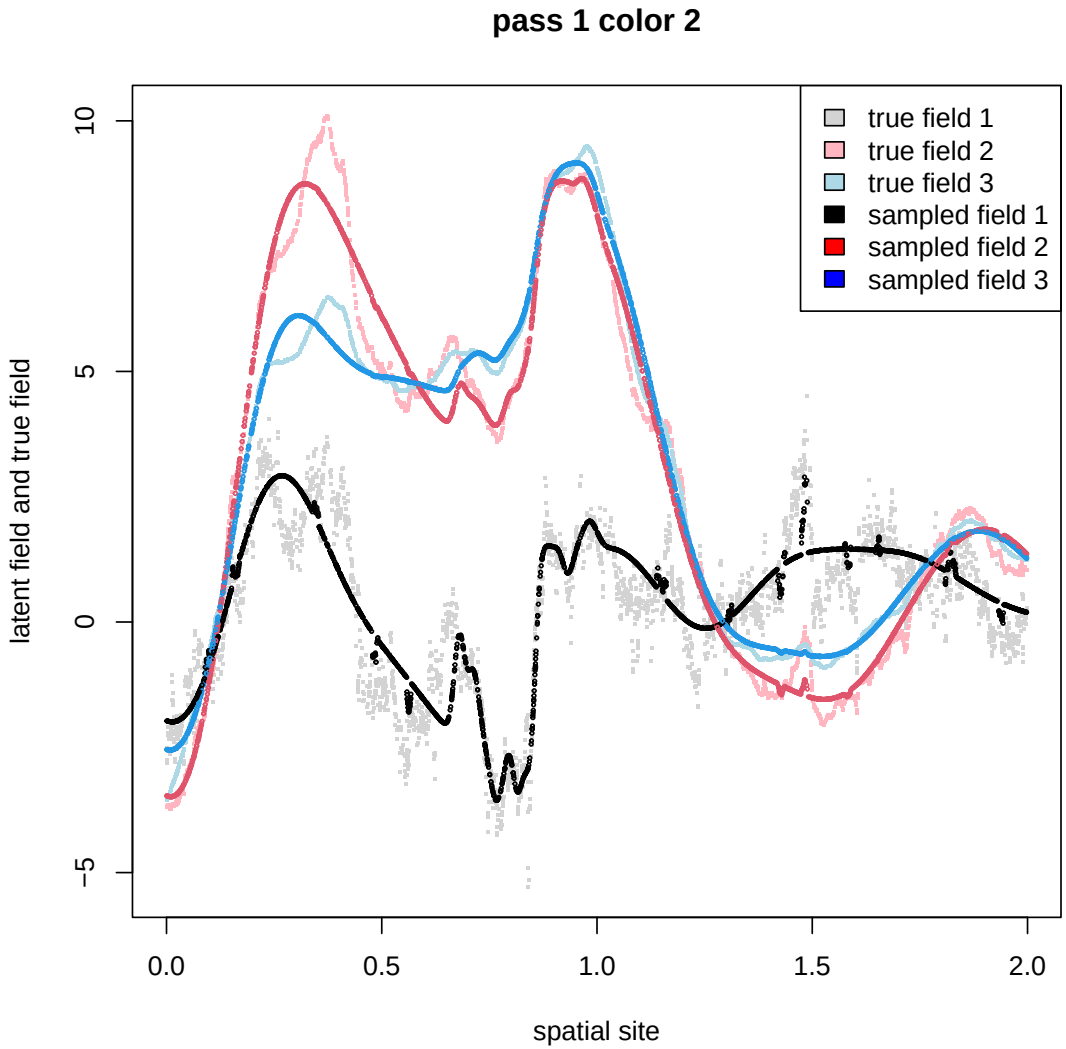

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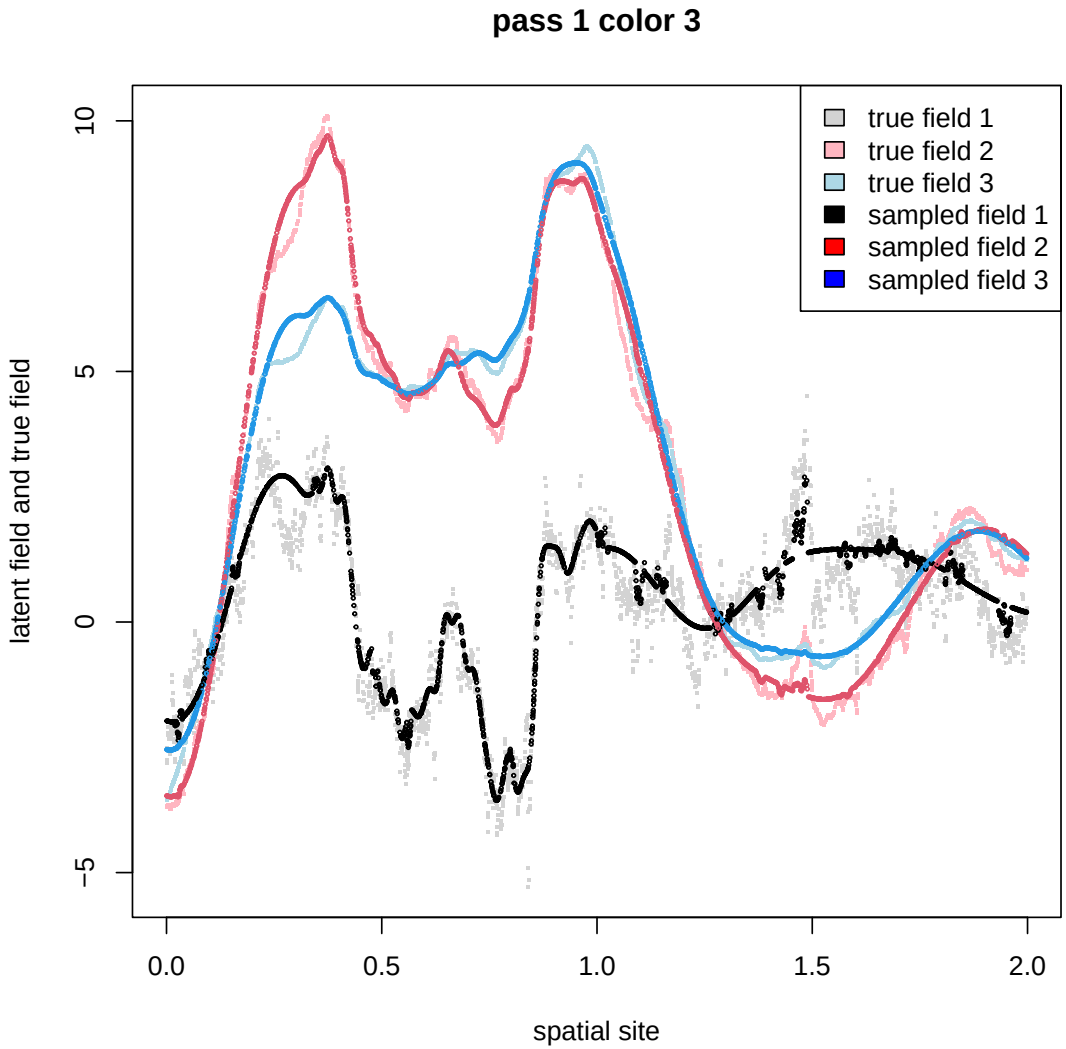

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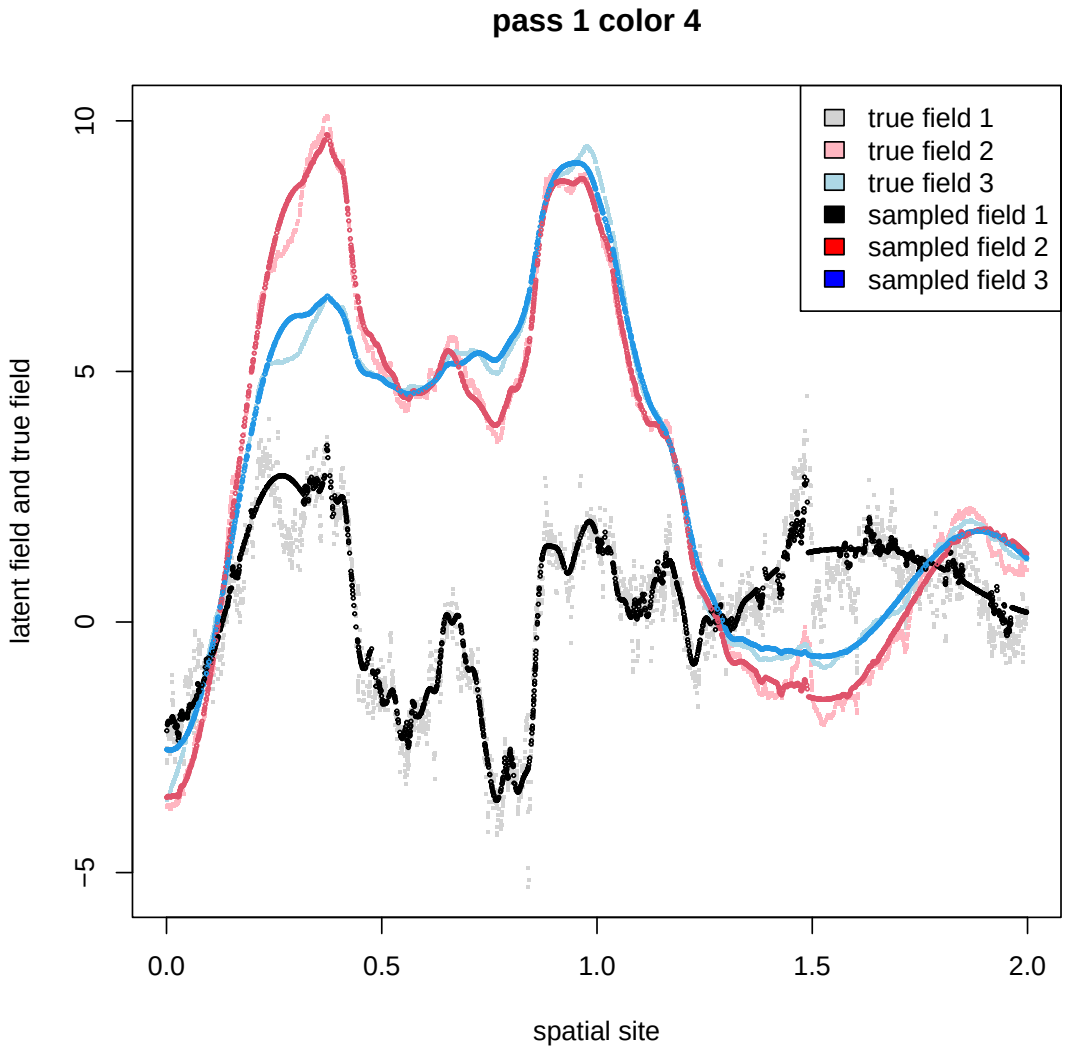

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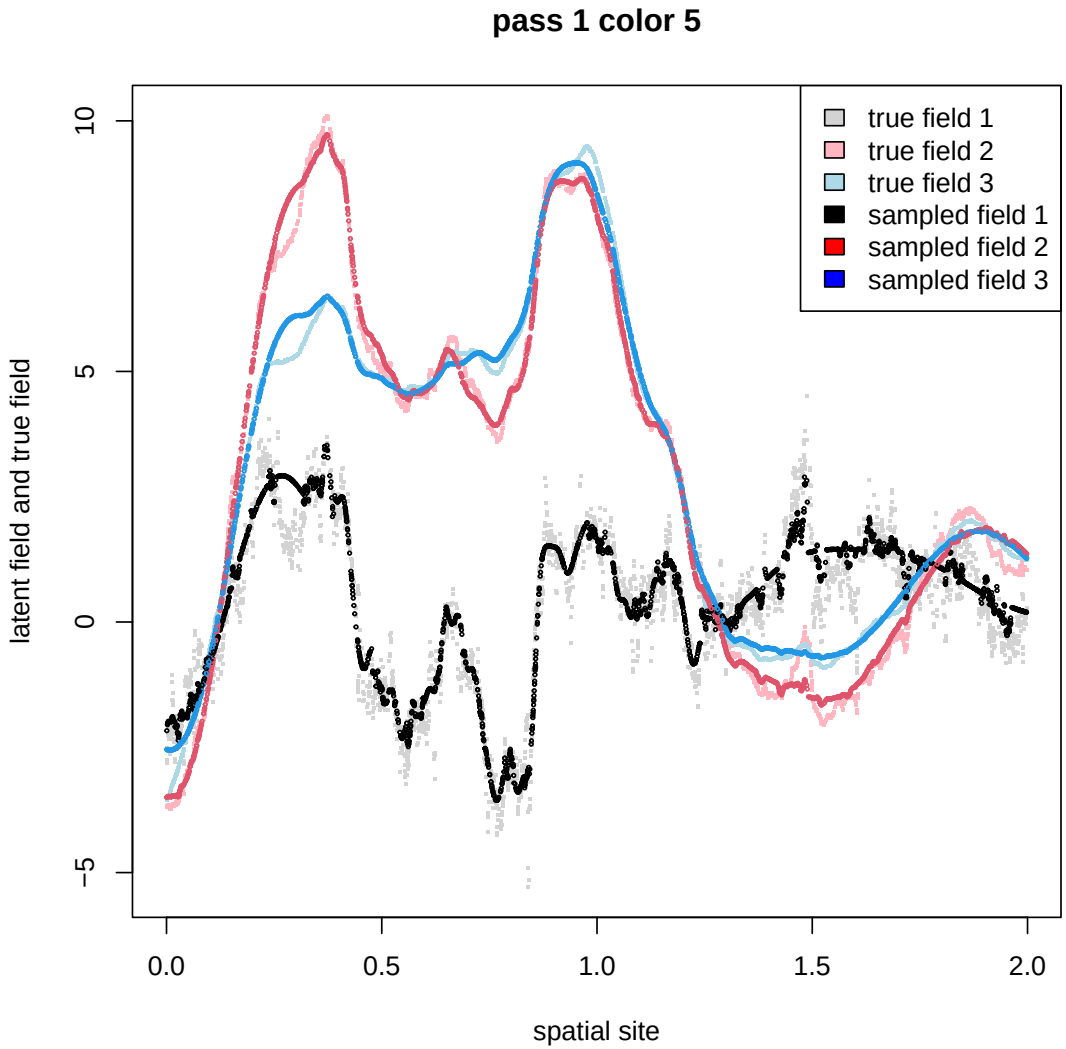

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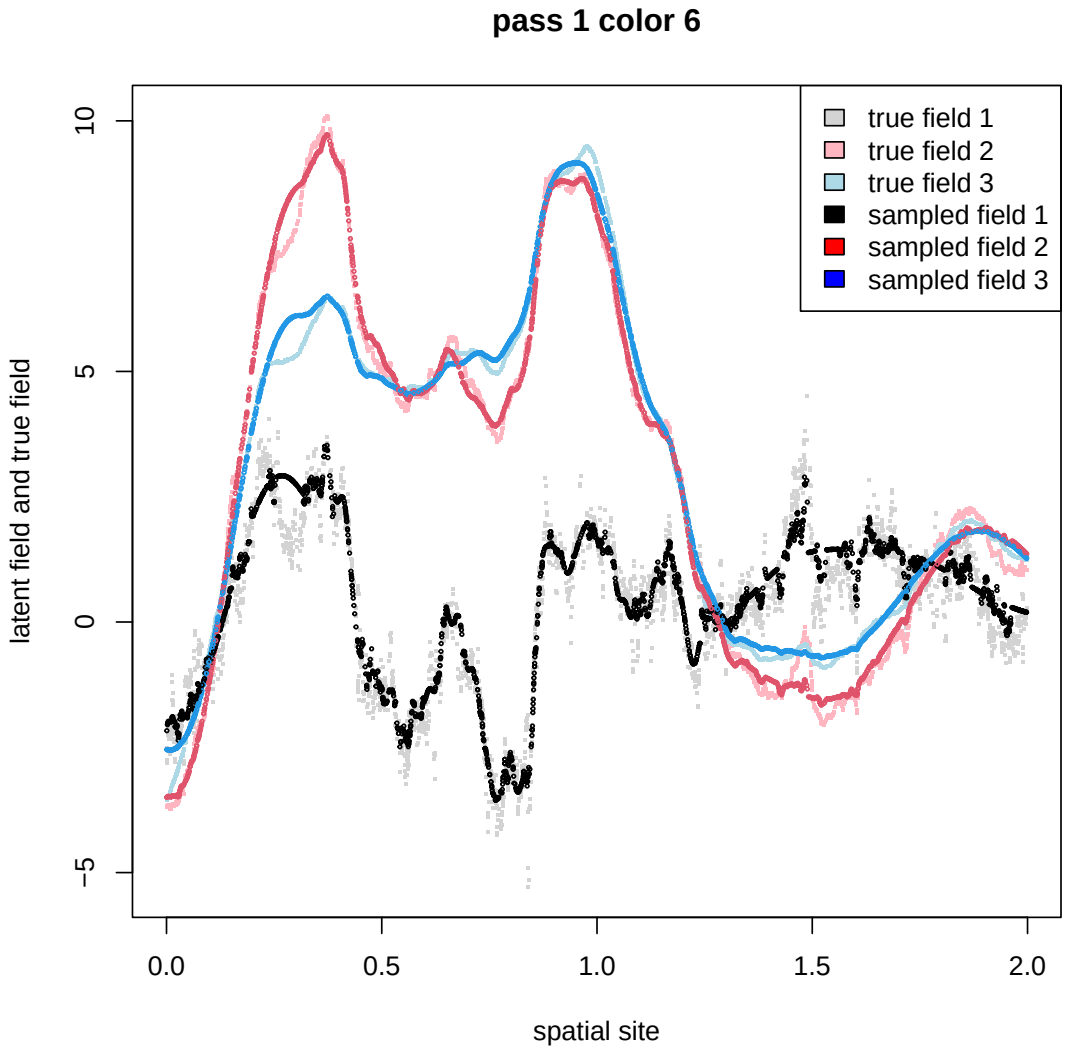

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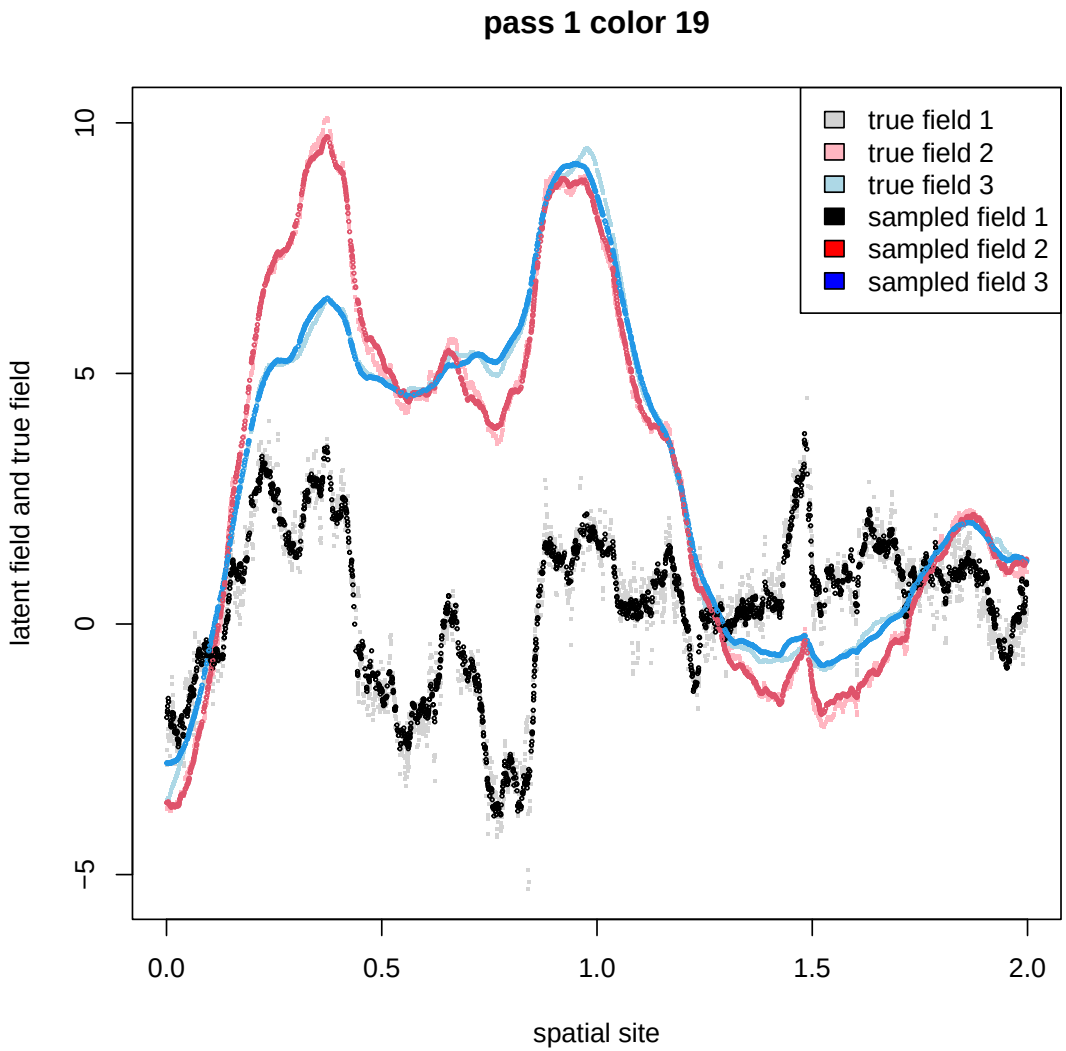

How does it run?

- Use of **parallelized** computing
- Moderate use of RAM

Figure 5: Sampling for a data set of 1.5 M observations

Bilbiography I

Allard, D., Clarotto, L., and Emery, X. (2022). Fully nonseparable gneiting covariance functions for multivariate space-time data.

Coube-Sisqueille, S. and Liquet, B. (2021). Improving performances of mcmc for nearest neighbor gaussian process models with full data augmentation. *Computational Statistics & Data Analysis*, page 107368.