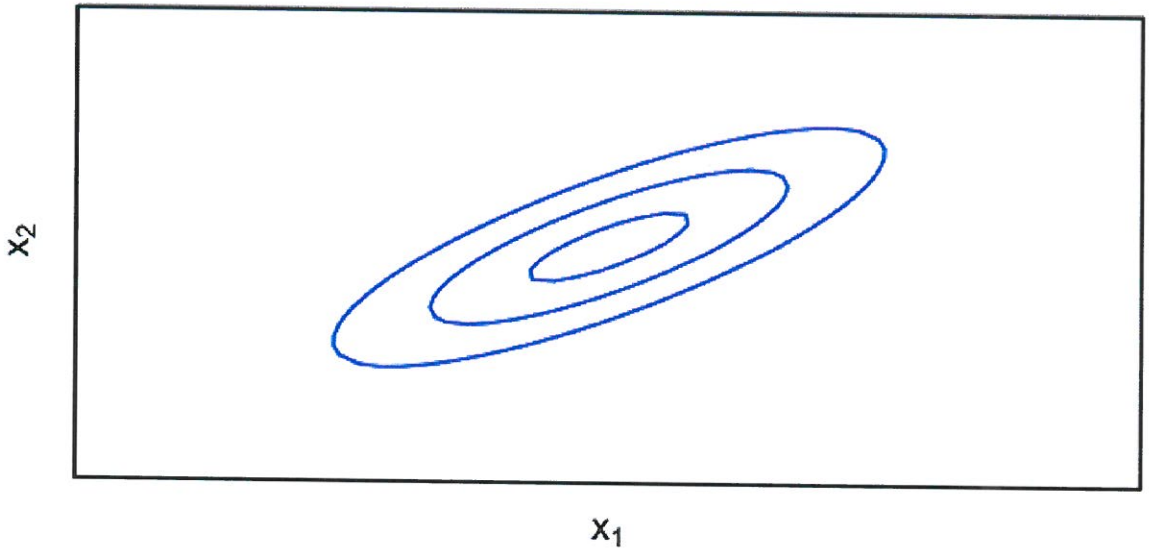
Multi-Fidelity Regression

with Gaussian Processes

Gaussian Distribution

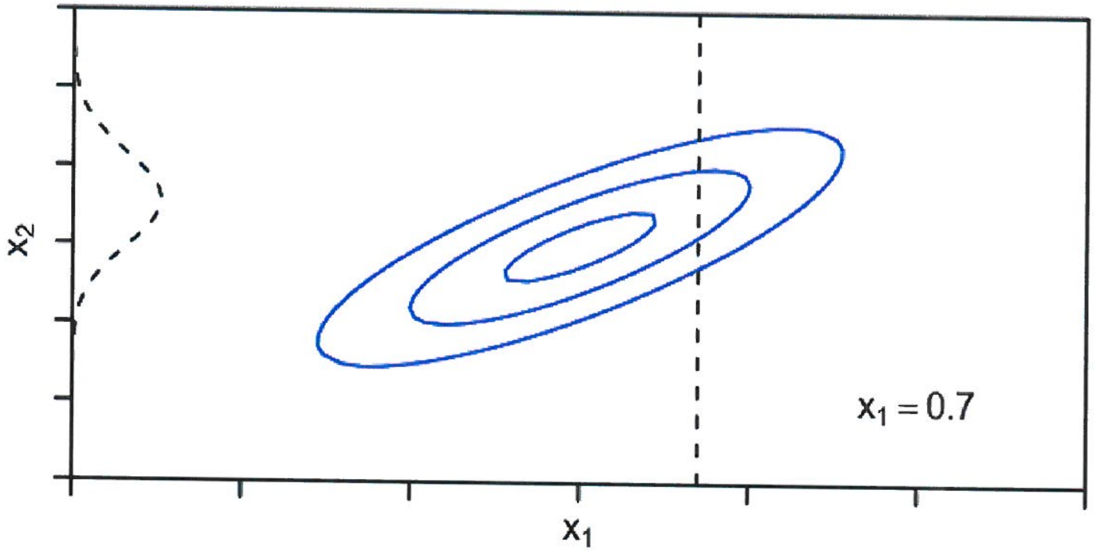
$$\frac{1}{\sqrt{2\pi|\Gamma|}} e^{-\frac{1}{2}(x-\mathbb{E}x)^T \Gamma^{-1} (x-\mathbb{E}x)}$$

$$\Gamma = \begin{bmatrix} 1 & .8 \\ .8 & 1 \end{bmatrix}$$

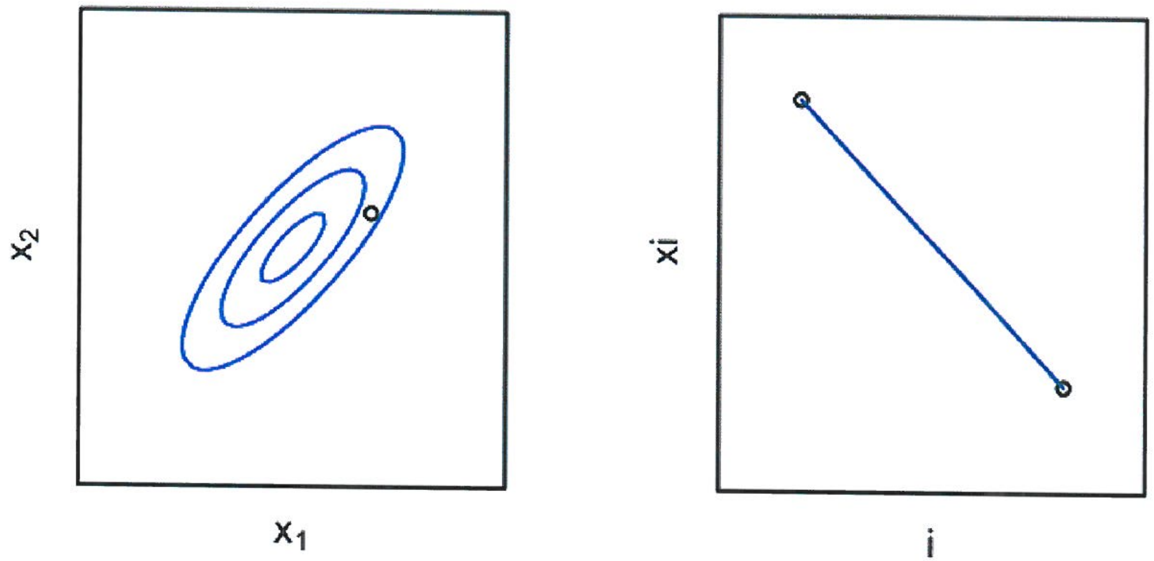


$$x_2 \mid x_1 = 0.7 \sim N(\mu_{x_2|x_1}, \Gamma_{x_2|x_1}) .$$

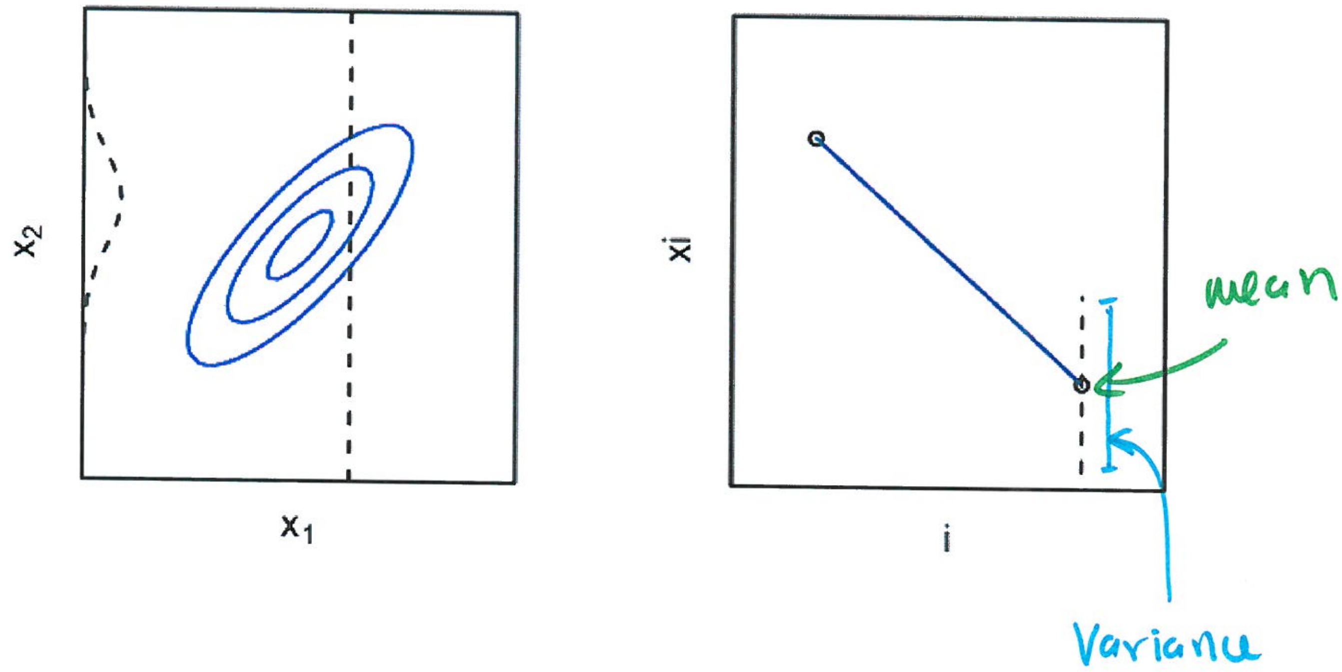
- $\mu_{x_2|x_1} = \mathbb{E}x_2 + \Gamma(x_2,x_1)\left(\Gamma(x_2,x_2)\right)^{-1} 0.7$
- $\Gamma_{x_2|x_1} = \Gamma(x_2,x_2) + \Gamma(x_2,x_1)\left(\Gamma(x_2,x_2)\right)^{-1}\Gamma(x_1,x_2)$



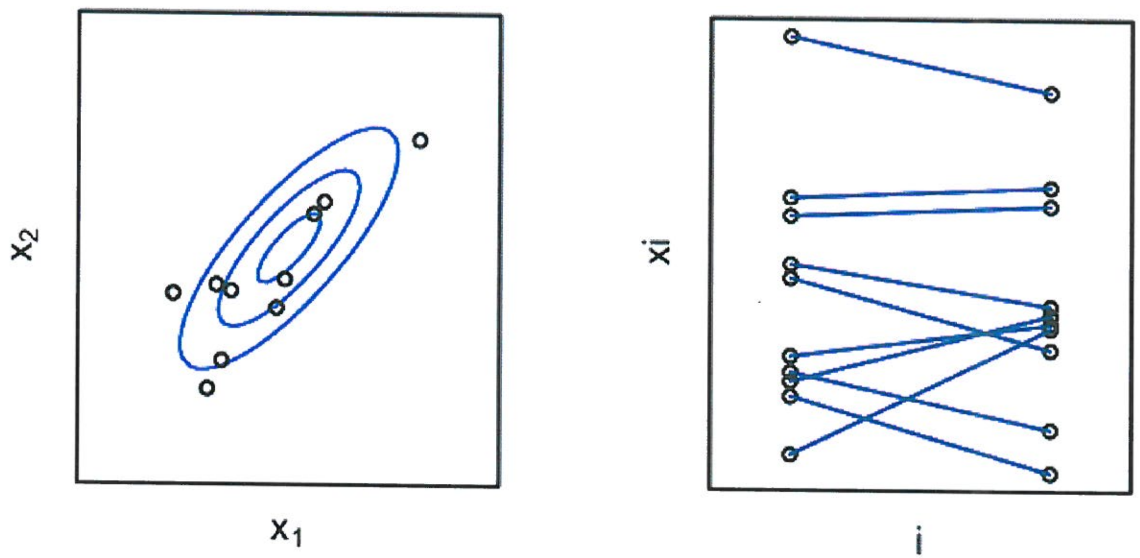
A convenient representation:



Same idea but for the conditional distribution.



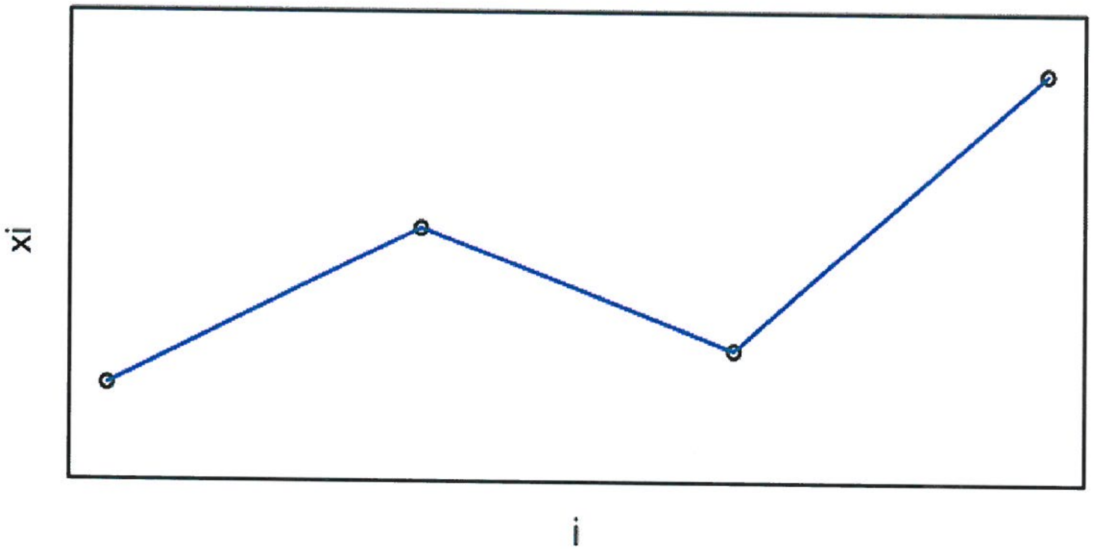
Many points look like:



Why? You can go to higher dimensions

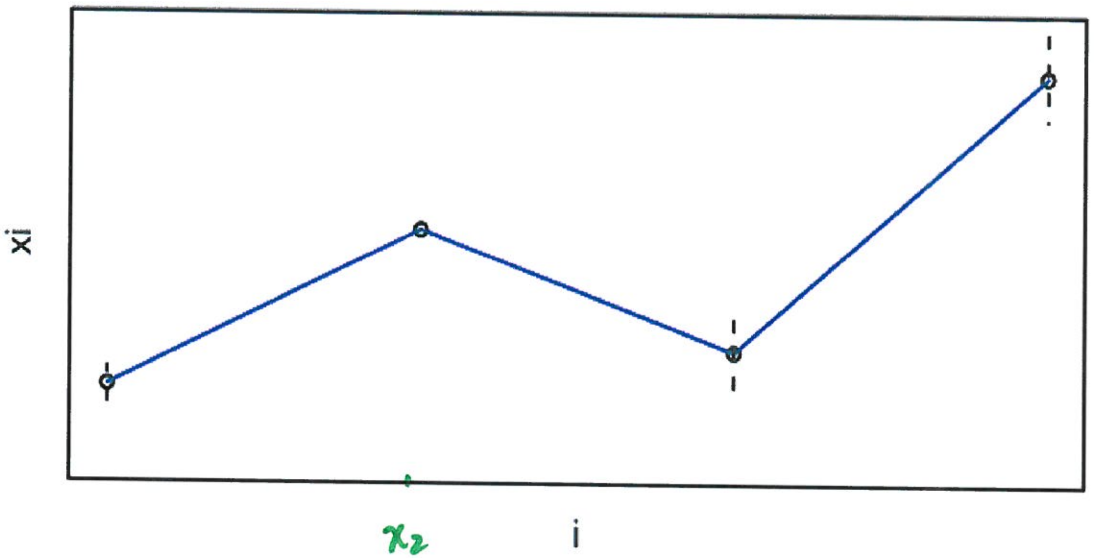
4 Dimensional Gaussian Vector (x_1, x_2, x_3, x_4)

$$\Gamma = \begin{bmatrix} 1 & .8 & .6 & .1 \\ .8 & 1 & .8 & .6 \\ .6 & .8 & 1 & .8 \\ .1 & .6 & .8 & 1 \end{bmatrix}$$

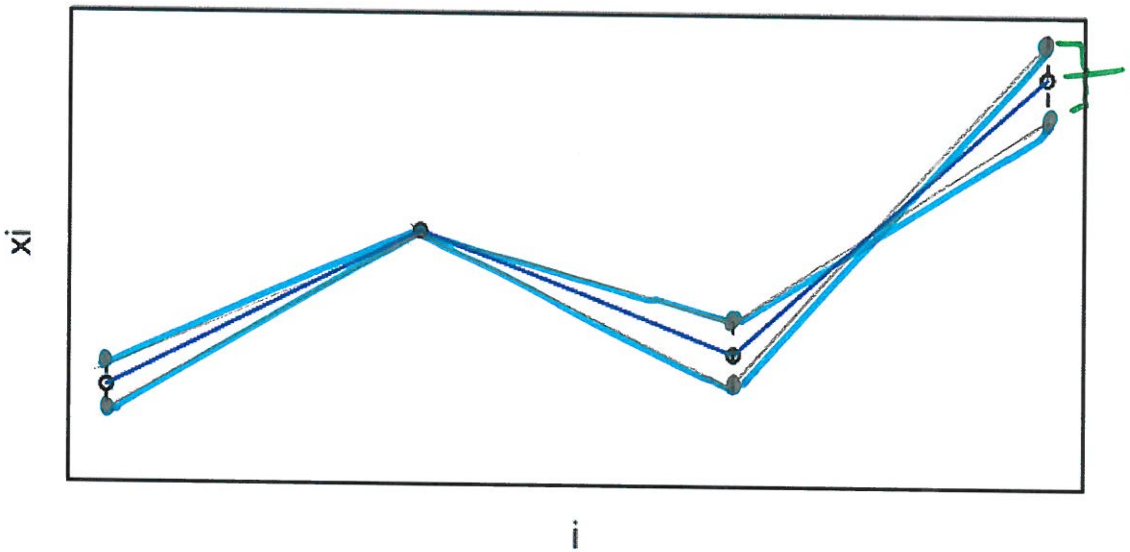


Conditional distribution.

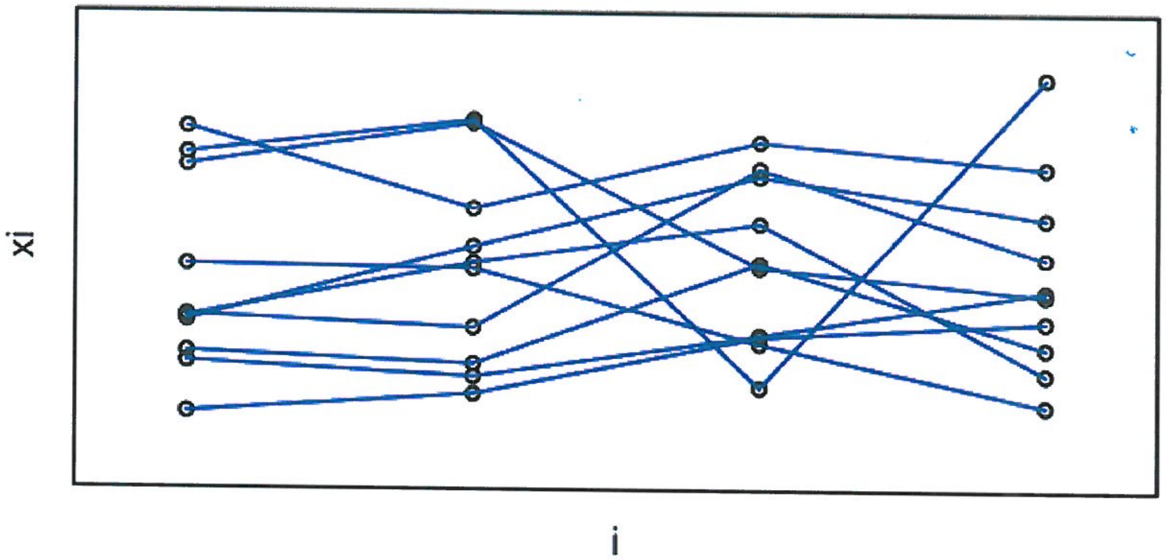
$X_1, X_3, X_4 \mid X_2 = x_2$



Sample from this conditional distribution.



Or from the whole space.



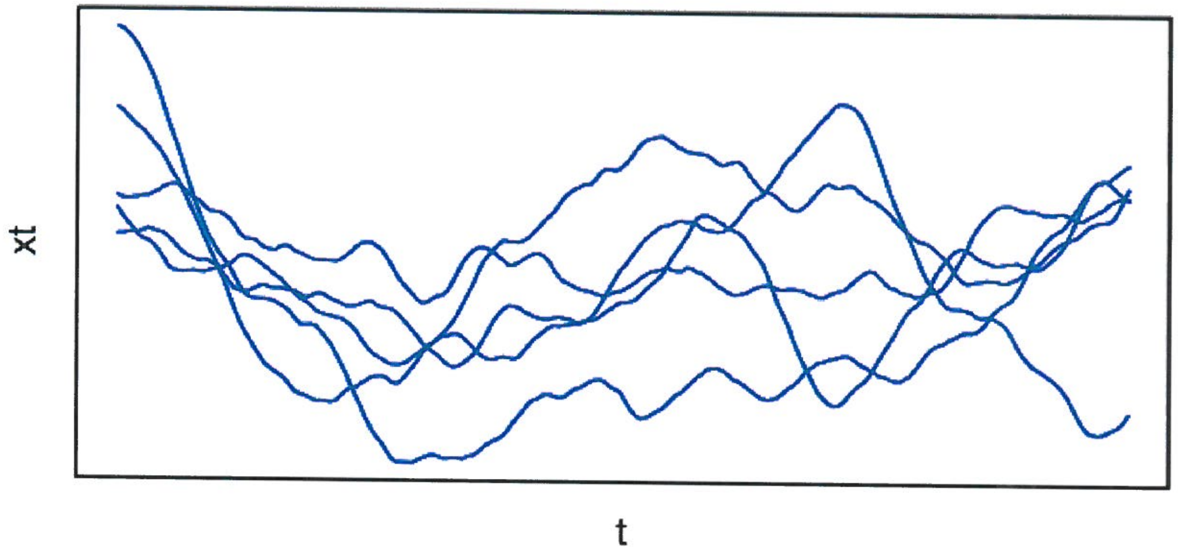
Gaussian process

mean function

$m(x_t) = \mu_t$

Covariance function

$\Gamma(x_t, x_s) = \sigma^2 \exp\left(-\frac{1}{2\ell^2}(t-s)^2\right)$

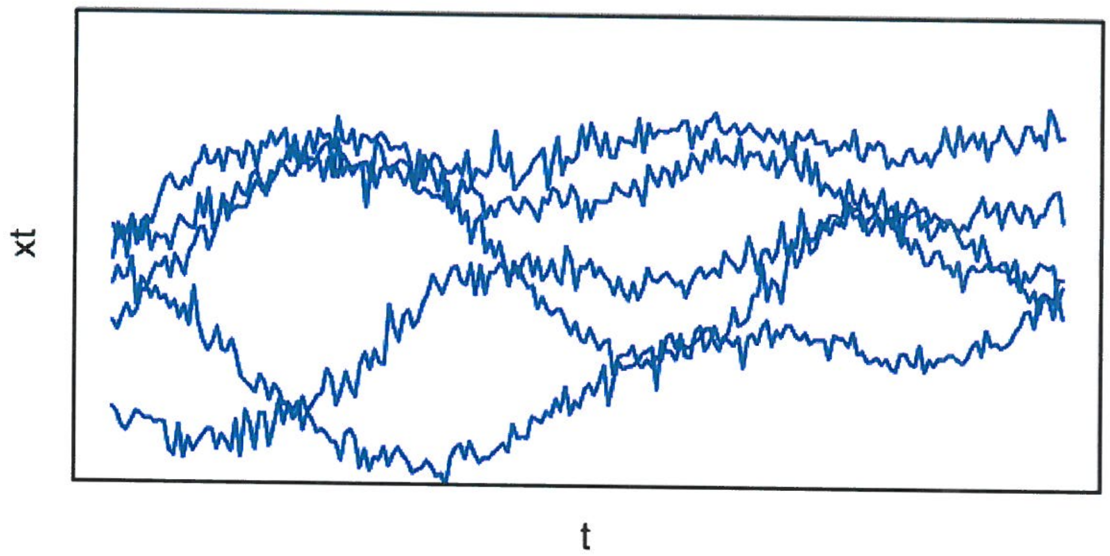


depends on

- ℓ^2
- σ^2

$$\Gamma(x_t, x_s) = \sigma^2 \exp\left(-\frac{1}{2\rho^2}|t-s|\right)$$

- Encode many properties through the cov. function.
  - Symmetries;
  - "Regularity";
  - Additivity.



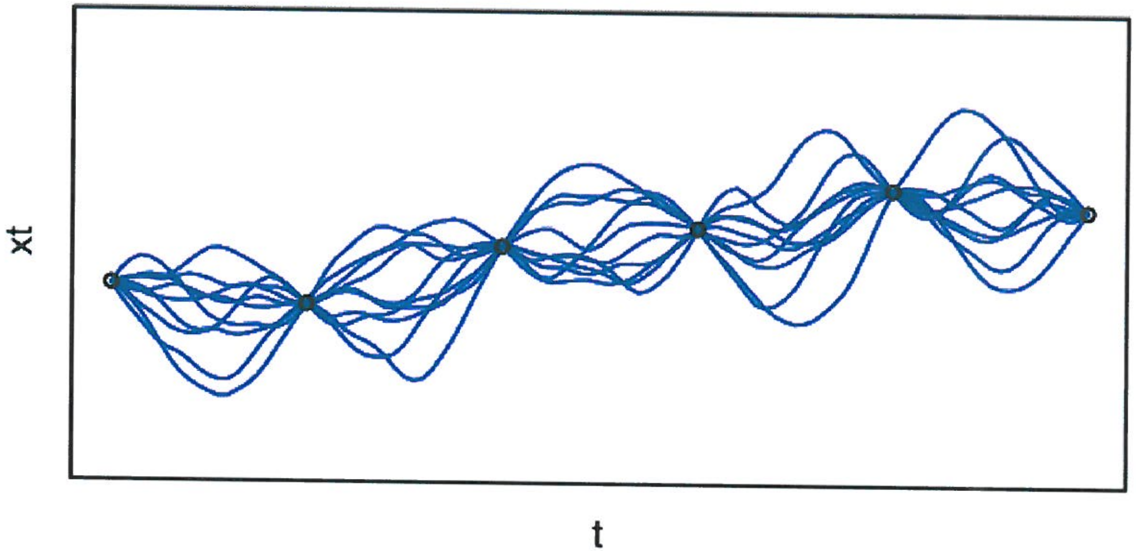
Notation

$$x_t \sim GP(m(x_t), \Gamma(x_t, x_s))$$

Conditional simulations.

Given the o's.

You can infere the parameters that define the covariance structure: l^2 and σ^2.



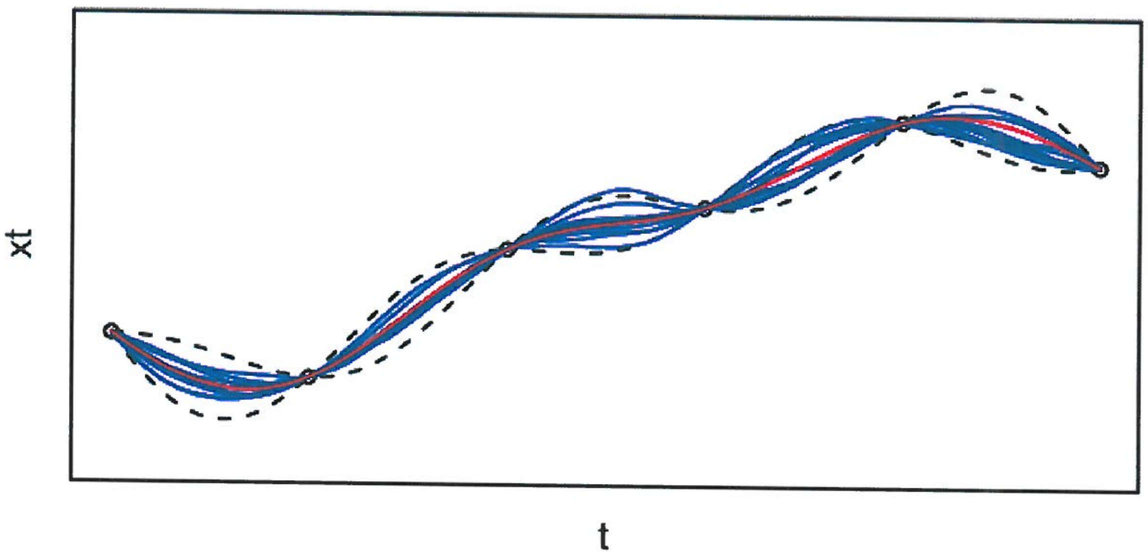
How? Likelihood (o's).

Use GP's to make predictions:

- Observe an unknown function: $h(t)$ at o.

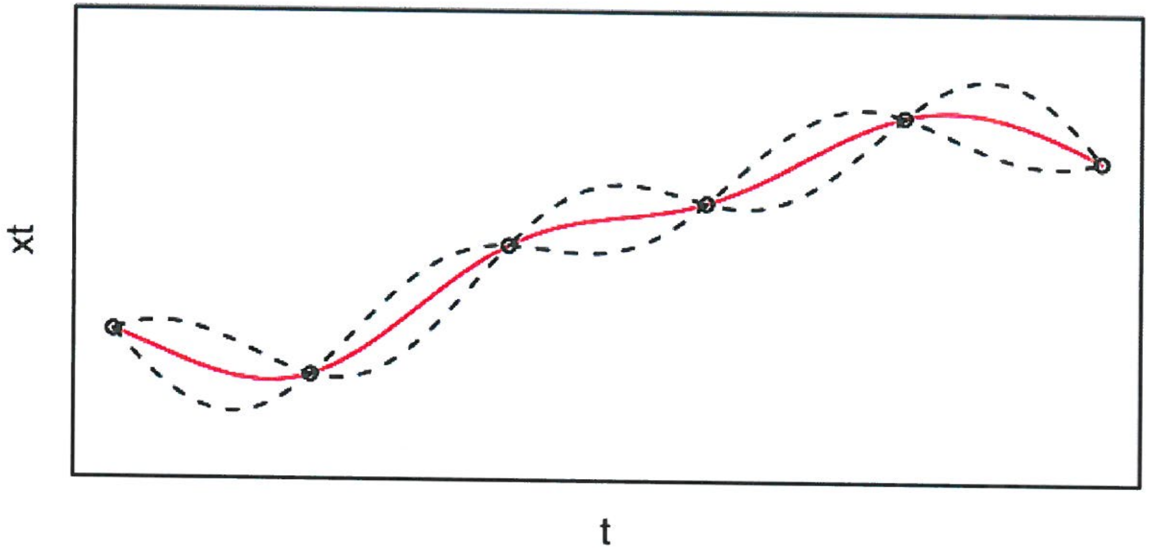
(1.) Use the obs to infre the parameters ℓ and σ^2.

(2.) Compute the conditional distribution.



Same representation as before

- The prediction at x_t is $\mathbb{E}[x_t \mid \text{Observed values}] =: \hat{x}_t$
- The prediction error is $\mathbb{E}[(x_t - \hat{x}_t)^2 \mid \text{Observed values}]$.



Multi-fidelity

- $X_{1,t} \sim GP\left(m_1(x_t), \Gamma_1(x_t, x_s)\right)$
- $X_{d,t} \sim GP\left(m_d(x_t), \Gamma_d(x_t, x_s)\right)$

$X_{1,t} \perp X_{d,s}$ for all s, and t.

$$\boxed{\begin{array}{l} X_{2,t} = g(t)\, X_{1,t} + X_{d,t} \\ \\ X_{2,t} = \varphi(X_{1,t}) + X_{d,t}. \end{array}}$$

or more generally

- Solving a PDE that depends on uncertain parameters

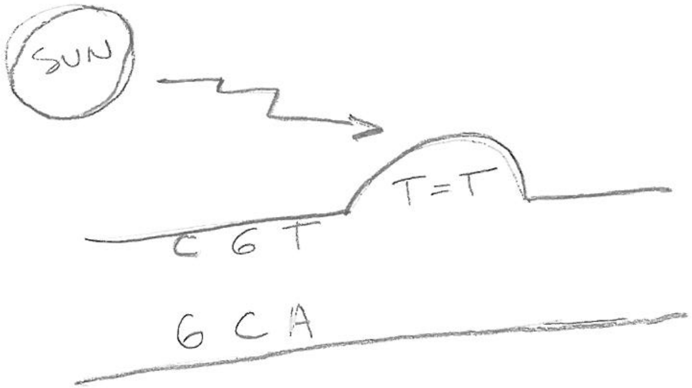
  $X_{2,t} \approx$ solution with a fine grid

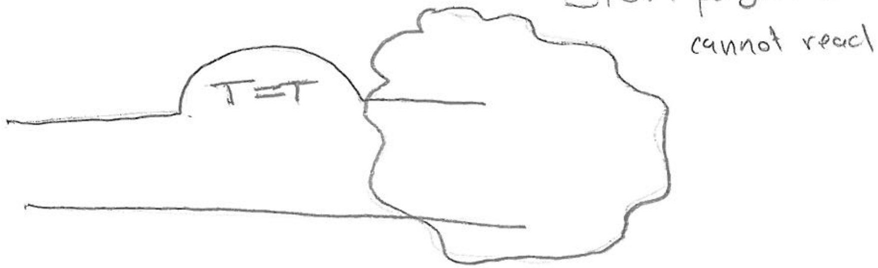
  $X_{1,t} \approx$ solution with a coarser grid.

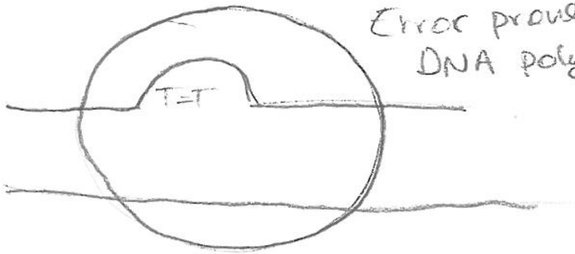
- We can compute $X_{1,t}$ for a large number of parameter combinations.

- To complement the few solutions of $X_{2,t}$.

Bacteries (are multi-fidelity?)







① UV mutation
[Rosemary Redfield UBC]

② [Rosemberg] E. Coli mutation manipulation

Damaged DNA gets repaired by Hi-fi / lo-fi polymerases.

lo-fi → errors in correction → mutations → survival.

Cipro: Damages DNA