Function factorization using warped Gaussian processes

Mikkel N. Schmidt

UNIVERSITY OF CAMBRIDGE

Computational and Biological Learning

Function factorization

- Non-linear regression
  - Input-output points, $\mathcal{D} = \{y^{(n)}, \boldsymbol{x}^{(n)}\}_{n=1}^{N}$
  - Regression function, $y : \mathcal{X} \to \mathbb{R}$
  - Predictions, $p(y^* | \boldsymbol{x}^*, \mathcal{D})$
- Key idea
  - Approximate

    complicated function on high-dimensional space
  - by sum of products of

    simpler functions on subspaces

Motivation

- Function factorization generalizes / combines
  - Matrix and tensor factorization
    Generalized multilinear model
  - Bayesian non-parametric regression
    Warped Gaussian process

Generalized multilinear model

- Describes data as factors
  - Add and multiply any combination of inputs

$$y_{i,j} = f_i^{(1,1)} f_j^{(1,2)} + f_i^{(2,1)} f_j^{(2,2)} + \cdots$$

- Flexible and interpretable

Function factorization model

Components

Factors

$$y(\boldsymbol{x}) = \sum_{k=1}^{K} \prod_{i=1}^{I} f^{(i,k)}(\boldsymbol{x}_i)$$

Output
$y \in \mathbb{R}$

Input
$\boldsymbol{x} \in \mathcal{X}$

Set of functions
$f^{(i,k)} : \mathcal{X}_i \rightarrow \mathbb{R}$

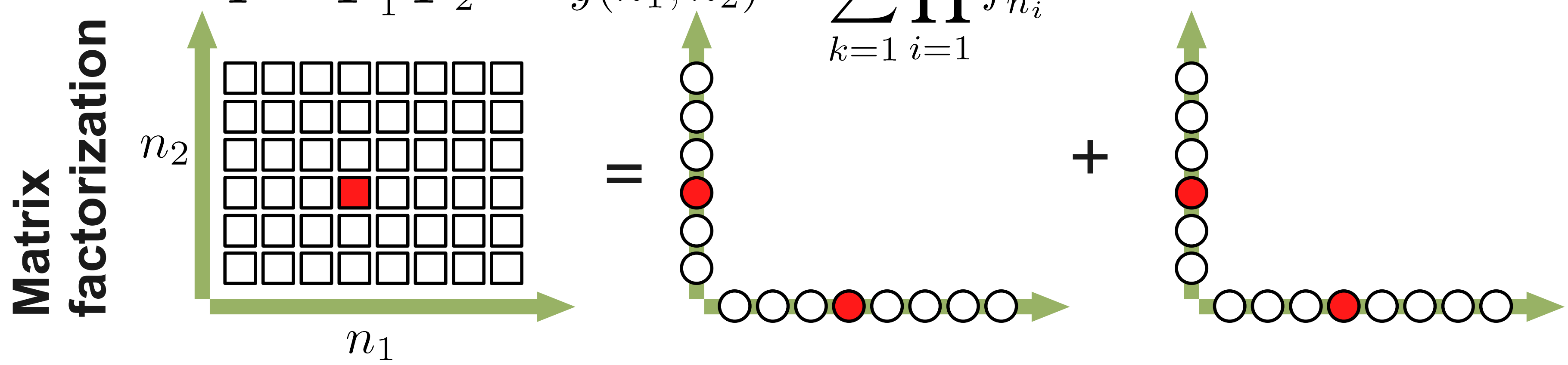
Input in subspace
$\boldsymbol{x}_i \in \mathcal{X}_i \subseteq \mathcal{X}$

Comparison to

Matrix factorization

$$\boldsymbol{Y} = \boldsymbol{F}_1^\top \boldsymbol{F}_2$$

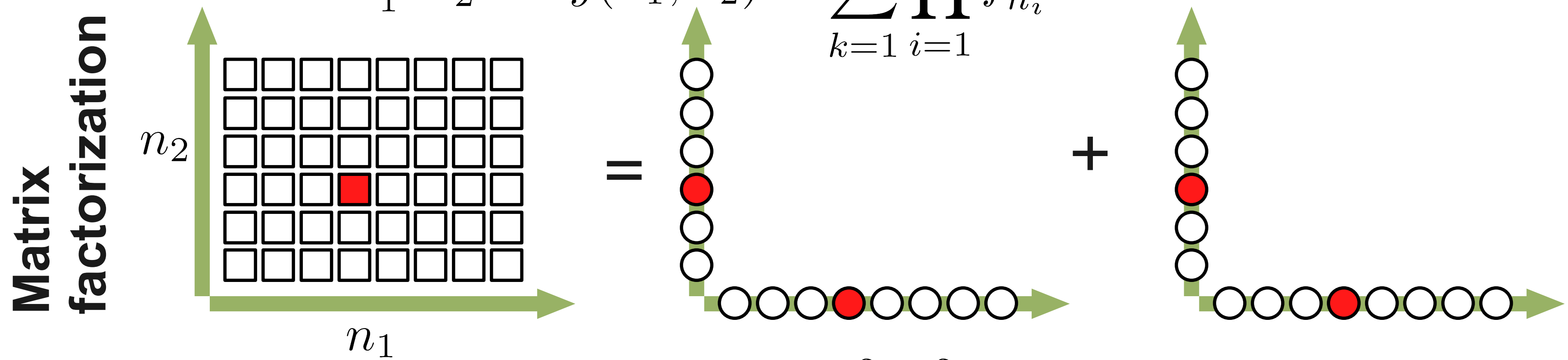
$$y(n_1, n_2) = \sum_{k=1}^{2} \prod_{i=1}^{2} f_{n_i}^{(i,k)}$$



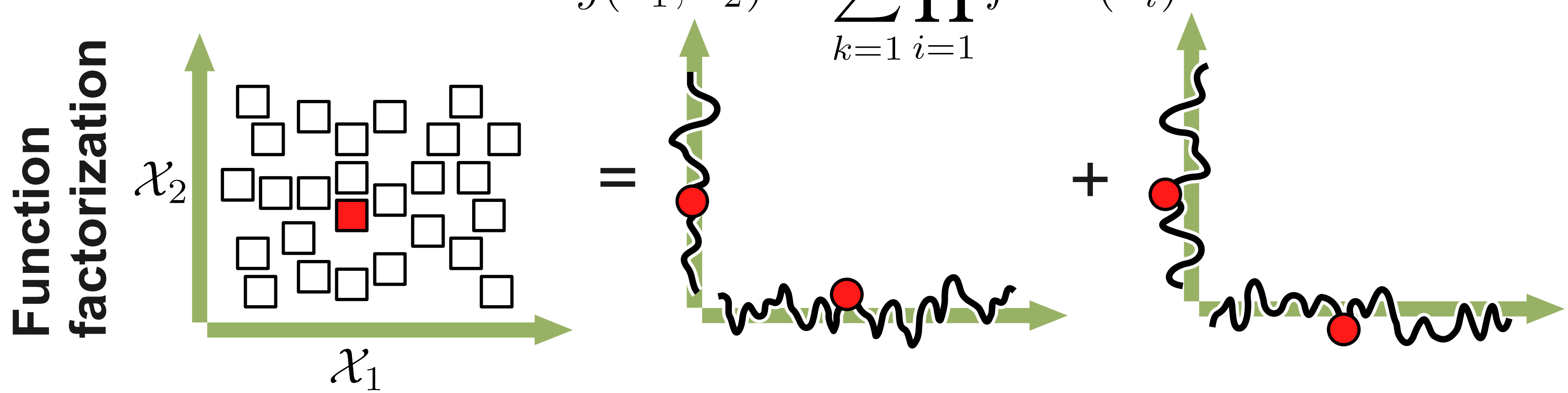
Comparison to

Matrix factorization

$$\boldsymbol{Y} = \boldsymbol{F}_1^\top \boldsymbol{F}_2 \qquad y(n_1, n_2) = \sum_{k=1}^{2} \prod_{i=1}^{2} f_{n_i}^{(i,k)}$$

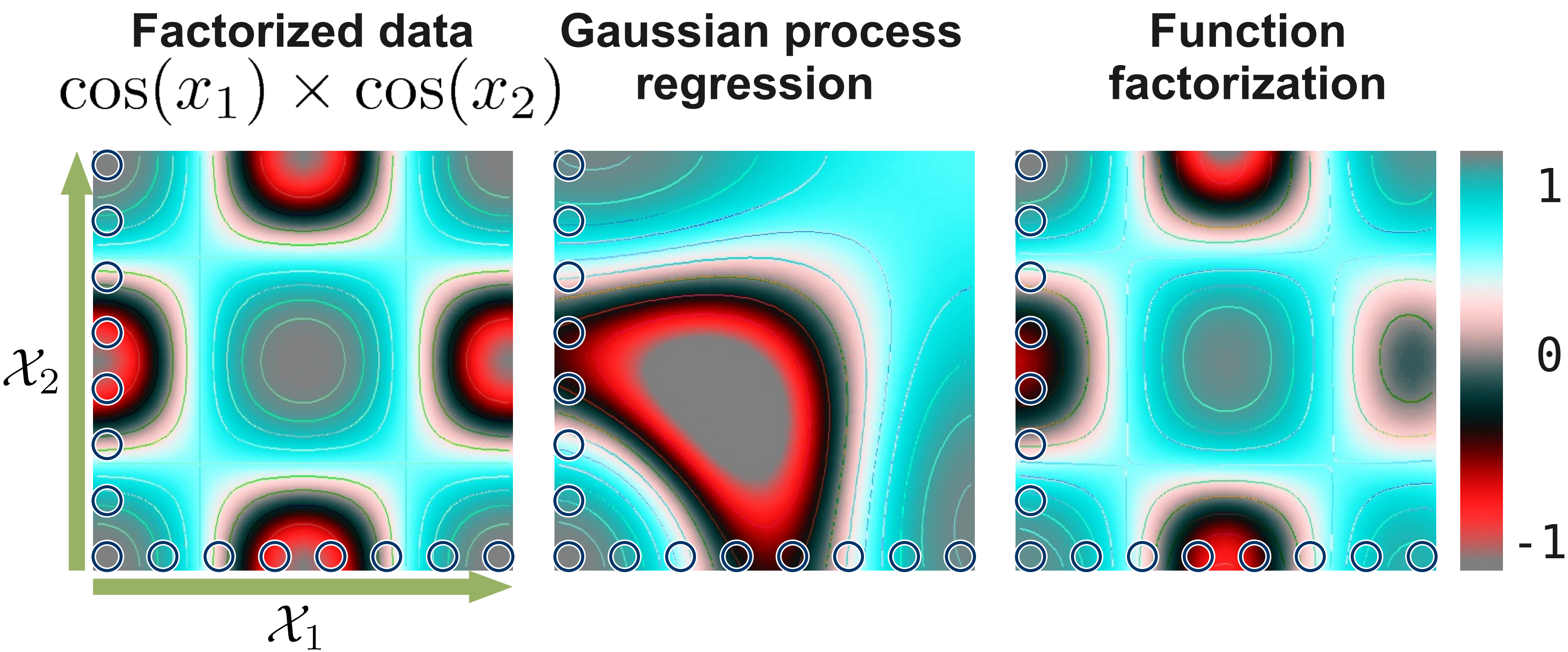


$$y(x_1, x_2) = \sum_{k=1}^{2} \prod_{i=1}^{2} f^{(i,k)}(x_i)$$



Comparison to

Gaussian process regression



Priors over functions

1) Parametric functions
   - Limited flexibility
2) Gaussian processes
   - Flexible and non-parametric
   - Limited by joint Gaussianity assumption
3) Warped Gaussian processes
   - GP warped by non-linear function

Warped Gaussian processes Snelson et al. (1999)

- GP warped by non-linear function

$$f(\boldsymbol{x}) = h(g(\boldsymbol{x})) \qquad g(\boldsymbol{x}) \sim \mathcal{GP}\big(m(\boldsymbol{x}), c(\boldsymbol{x}, \boldsymbol{x}')\big)$$

Non-linear warp function

Gaussian process

Mean function

Covariance function

- Parameters of warp and covariance functions are learned from data

Inference

- Hamiltonian Markov chain Monte Carlo
  Duane et al. (1987)
- Integrate out all parameters
  - Likelihood function (noise variance)
  - GP latent variables
  - Covariance functions
  - Warp functions
- Gradients wrt. all parameters

Color of beef data

Bro and Jakobsen (2002)

Color of beef as it changes during storage

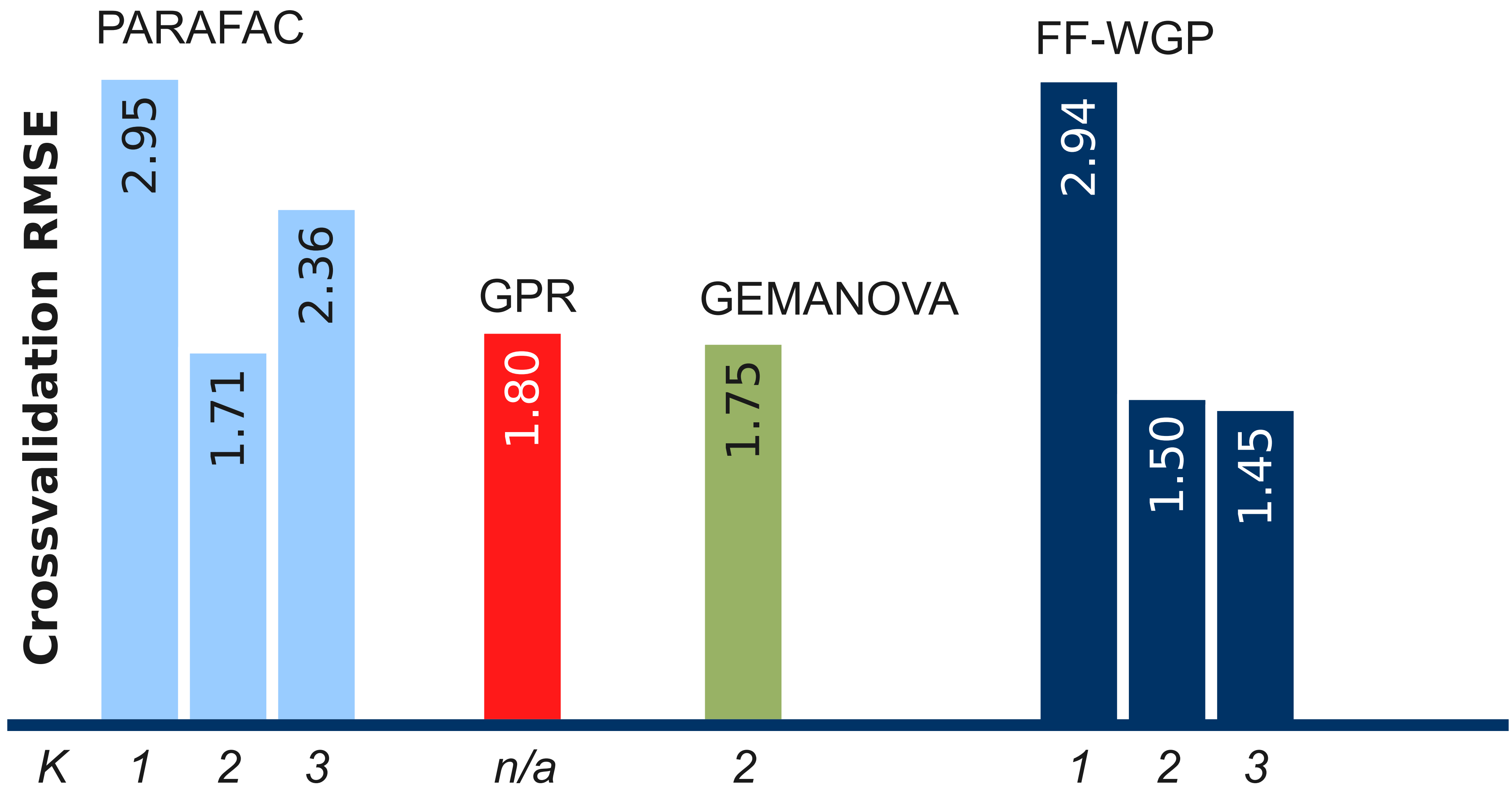
- Storage time
- Temperature
- Oxygen content
- Exposure to light

Task: Predict color from condition

Color of beef data

- Data: 5-way array
  - Measured red color on non-negative scale
- 60% missing val
  - PARAFAC: Handle missing data using EM iterations
  - Function factorization: Does not require data on grid
- Warp function
  - Parameterized function that maps to the non-negative numbers

Results



PARAFAC
GPR
GEMANOVA
FF-WGP
Crossvalidation RMSE
2.95
1.71
2.36
1.80
1.75
2.94
1.50
1.45
K
1
2
3
n/a
2
1
2
3

Summary

- New approach to non-linear regression
- Generalizes matrix and tensor factorization
- Exploits factorized structure in data
- Warped Gaussian process priors over functions
- Bayesian inference (Hamiltonian Monte Carlo)
  - Integrate out all parameters
- Outperforms PARAFAC and GPR

References

Bro and Jakobsen (2002), Exploring complex interactions in designed data using GEMANOVA. Color changes in fresh beef during storage. Chemometrics, Journal of, 16, 294–304.

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