Fast Discovery of Pairwise Interactions in High Dimensions using Bayes

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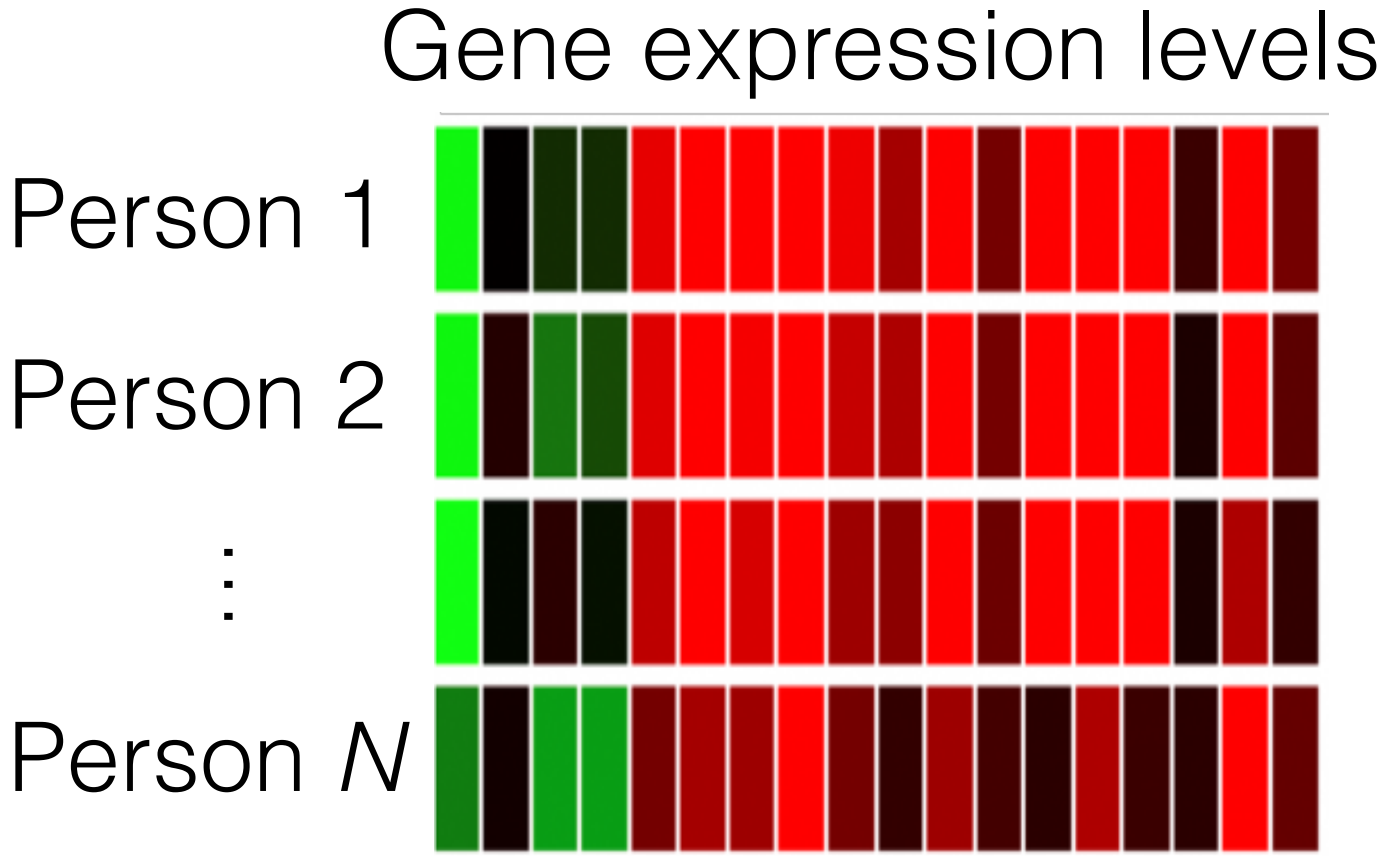
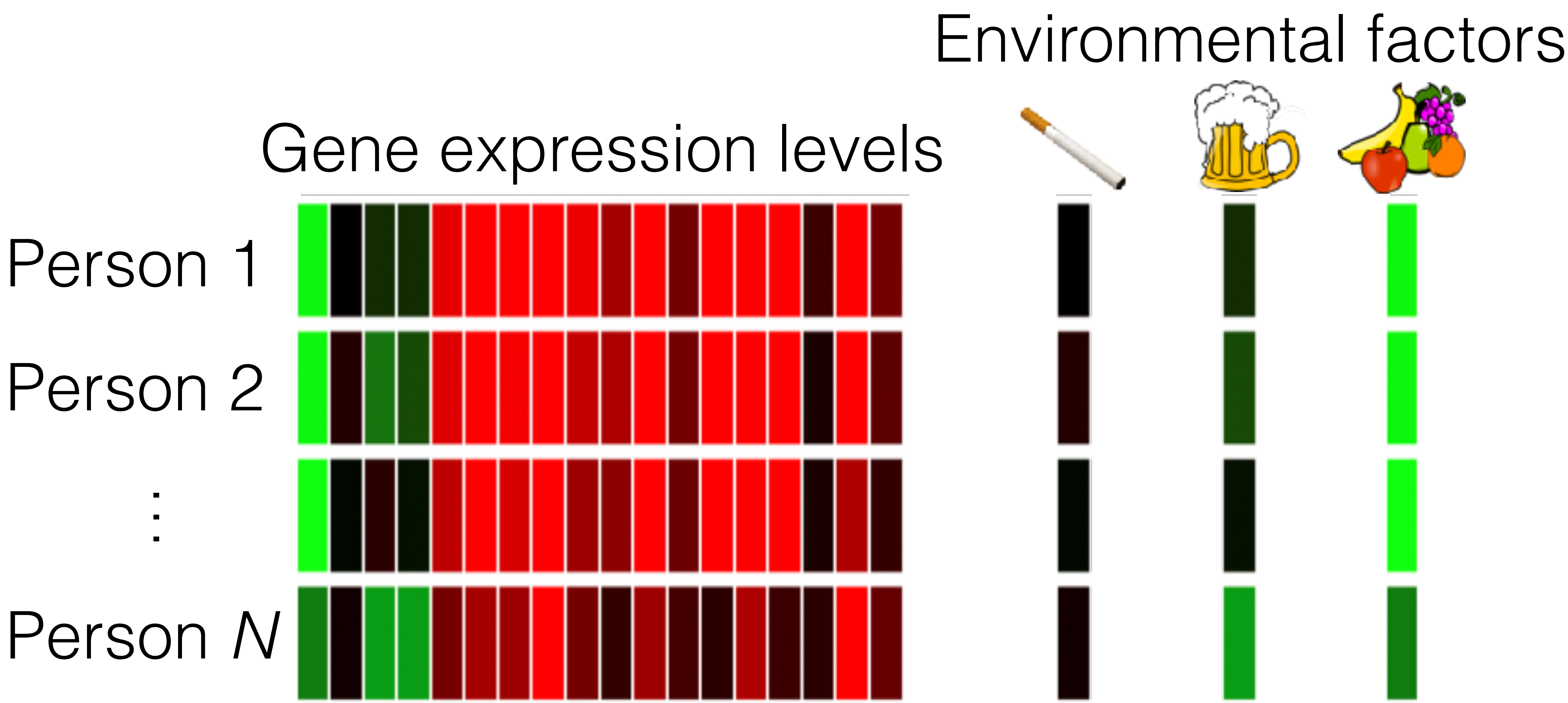
Associate Professor
EECS, MIT

Raj Agrawal, Jonathan H. Huggins, Brian L. Trippe




Gene expression levels
Person 1
Person 2
⋮
Person N


Environmental factors
Gene expression levels
Person 1
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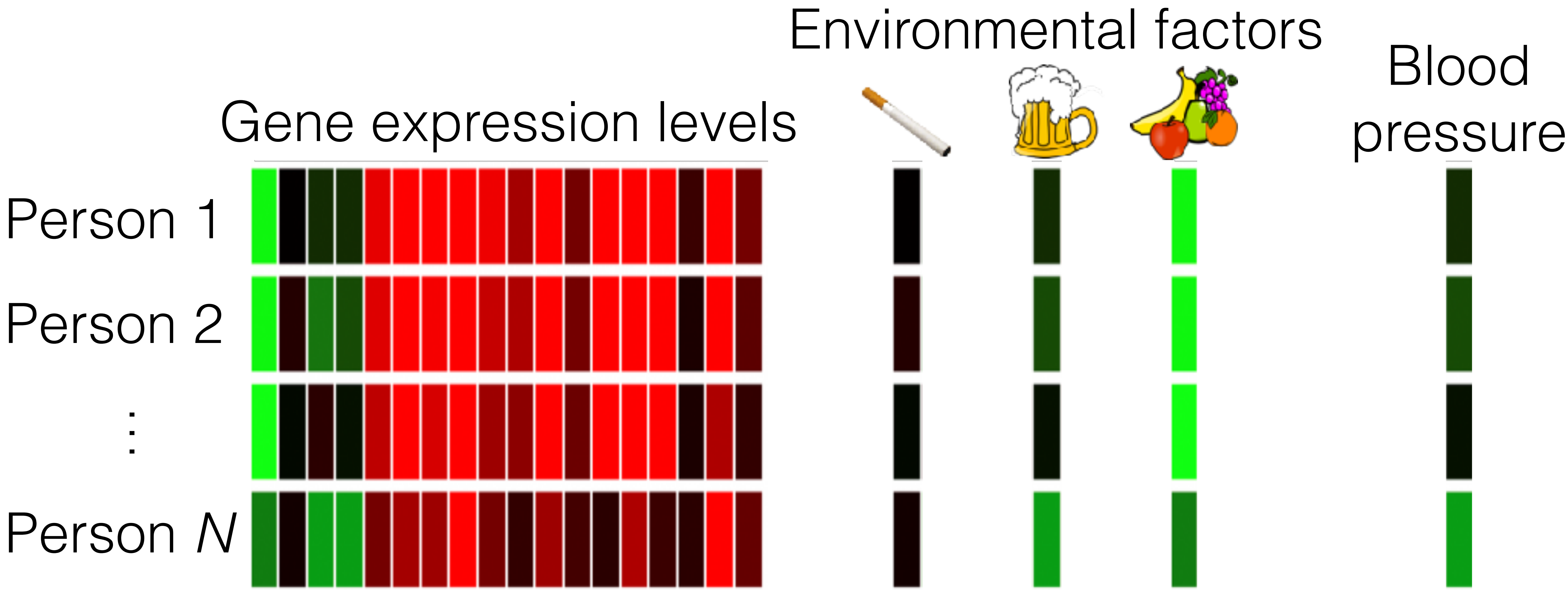
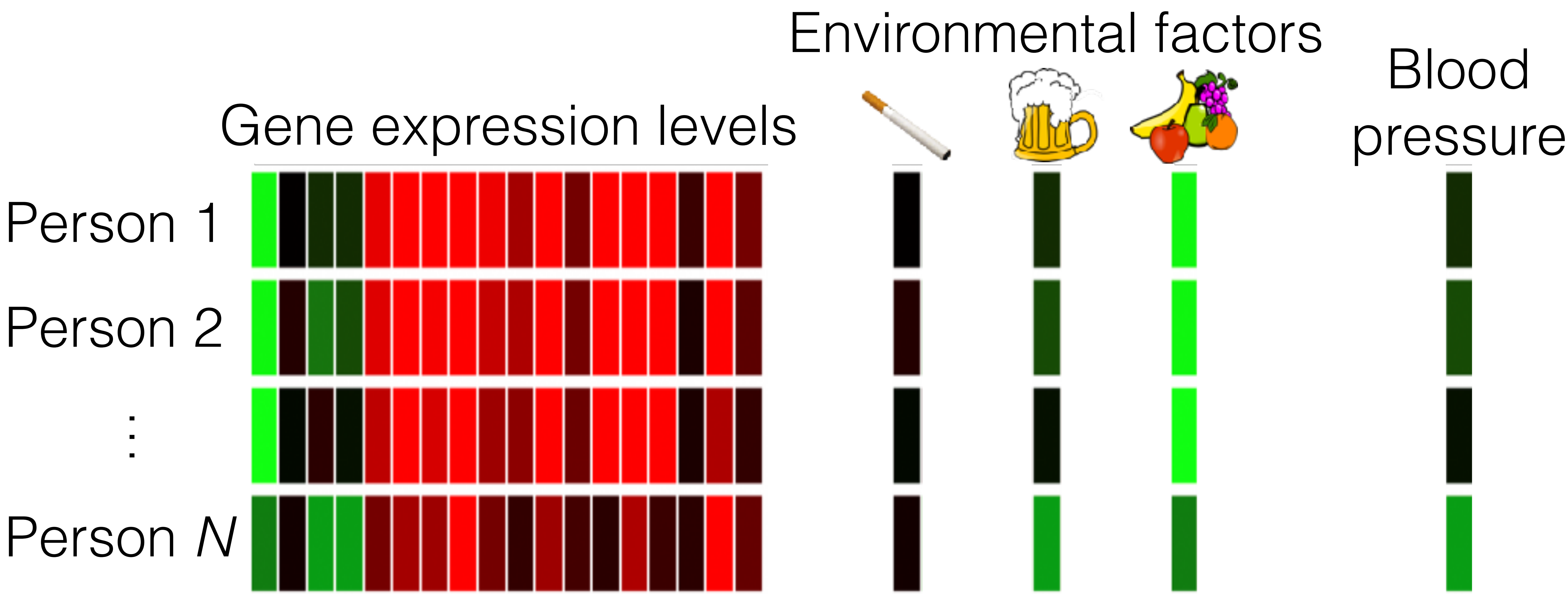
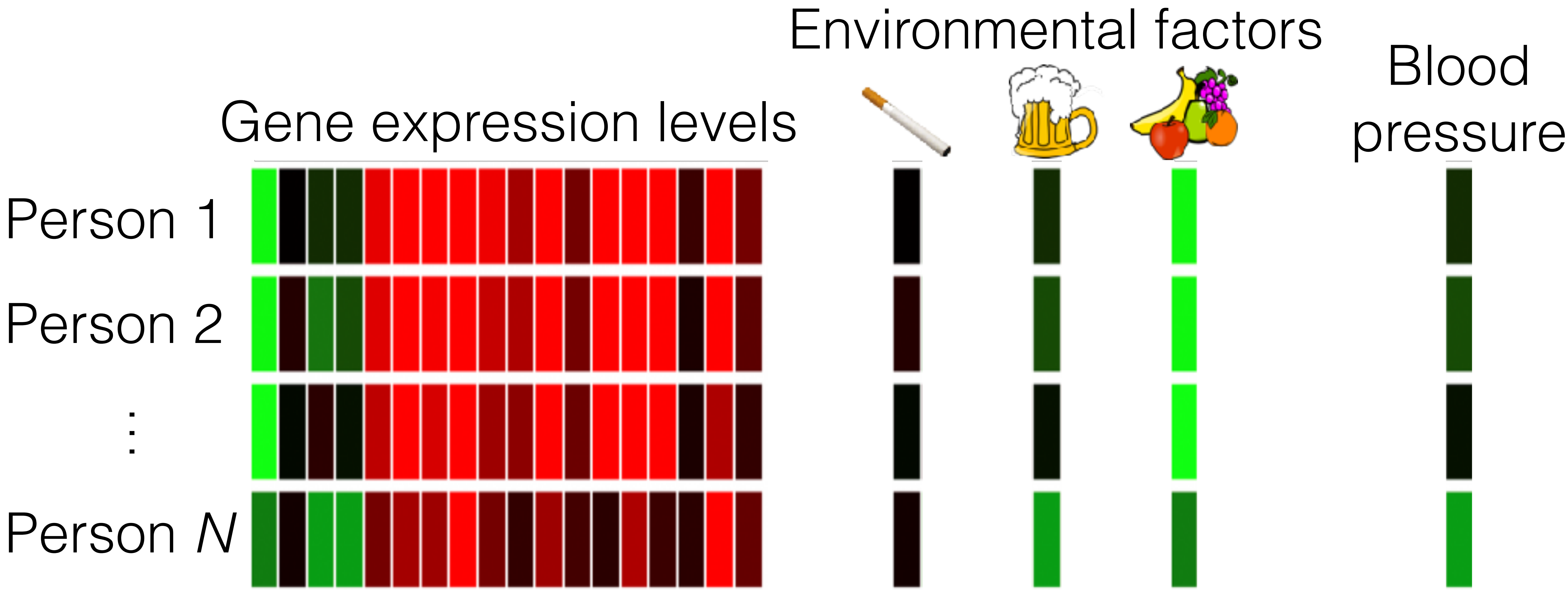
⋮
Person N


Environmental factors
Blood pressure
Gene expression levels
Person 1
Person 2
⋮
Person N



- Which genes/factors are associated with a health issue?



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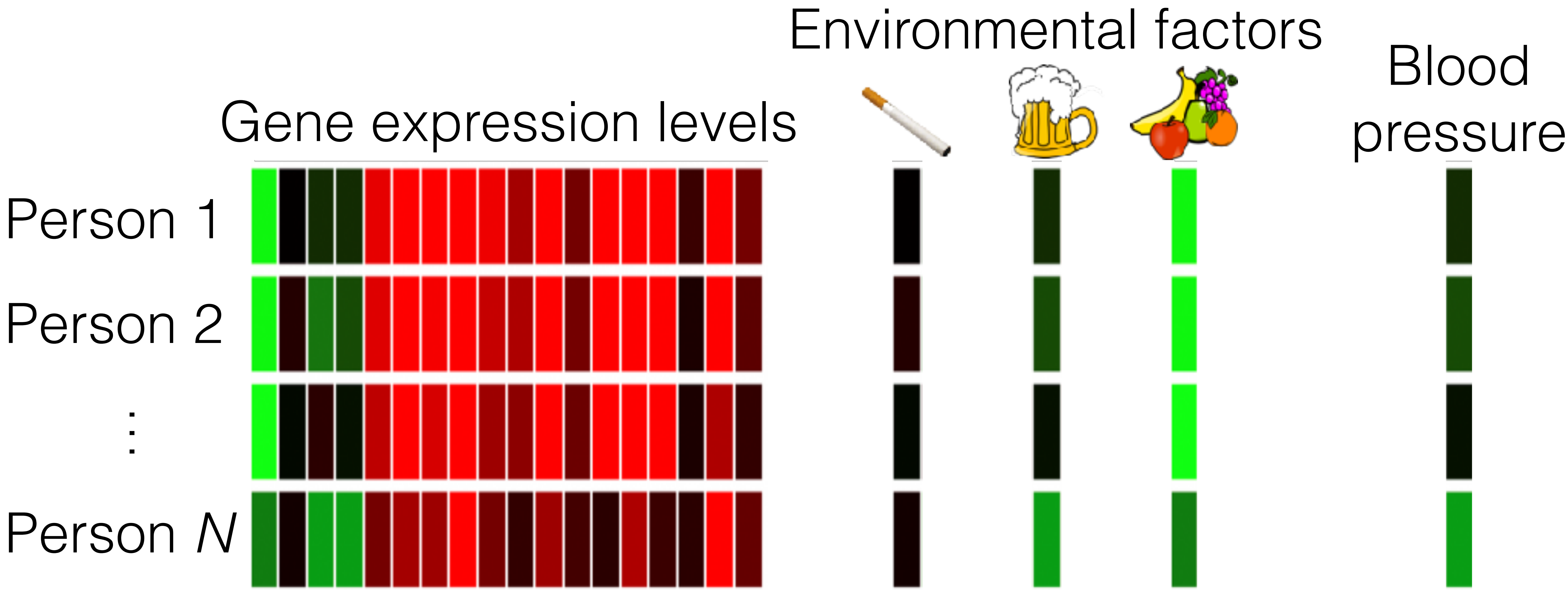

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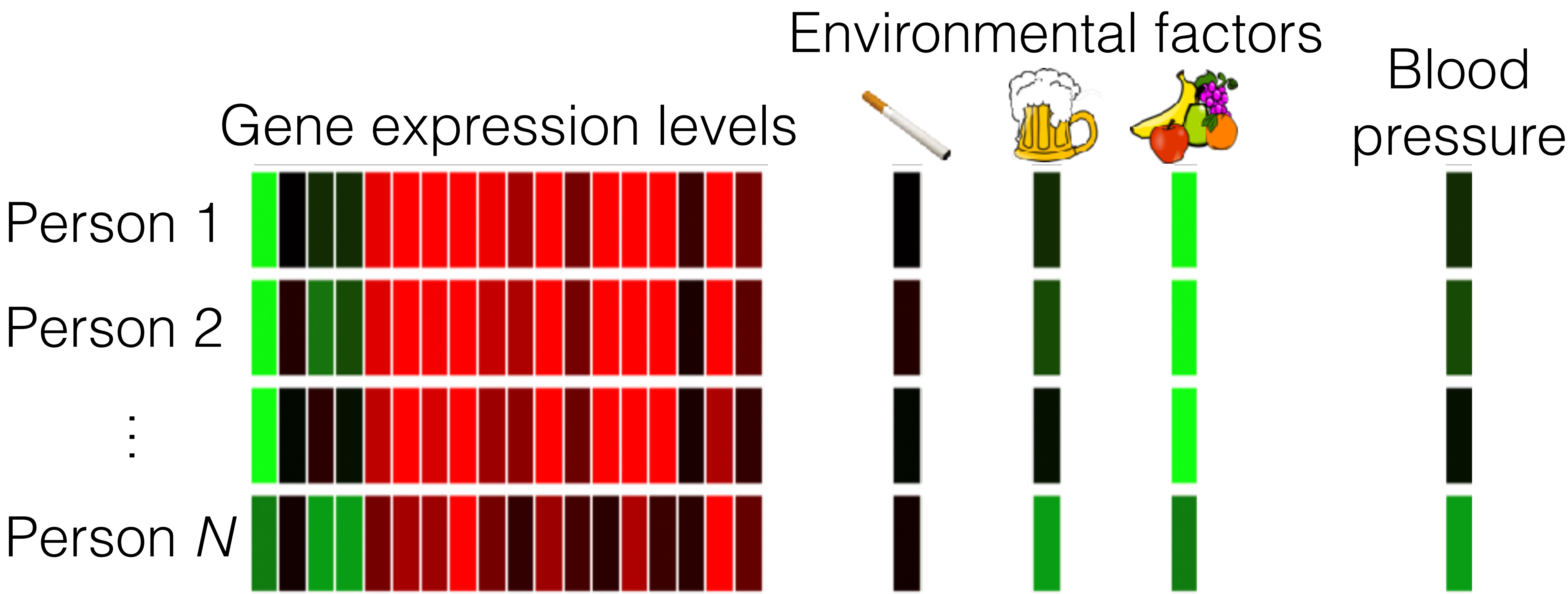

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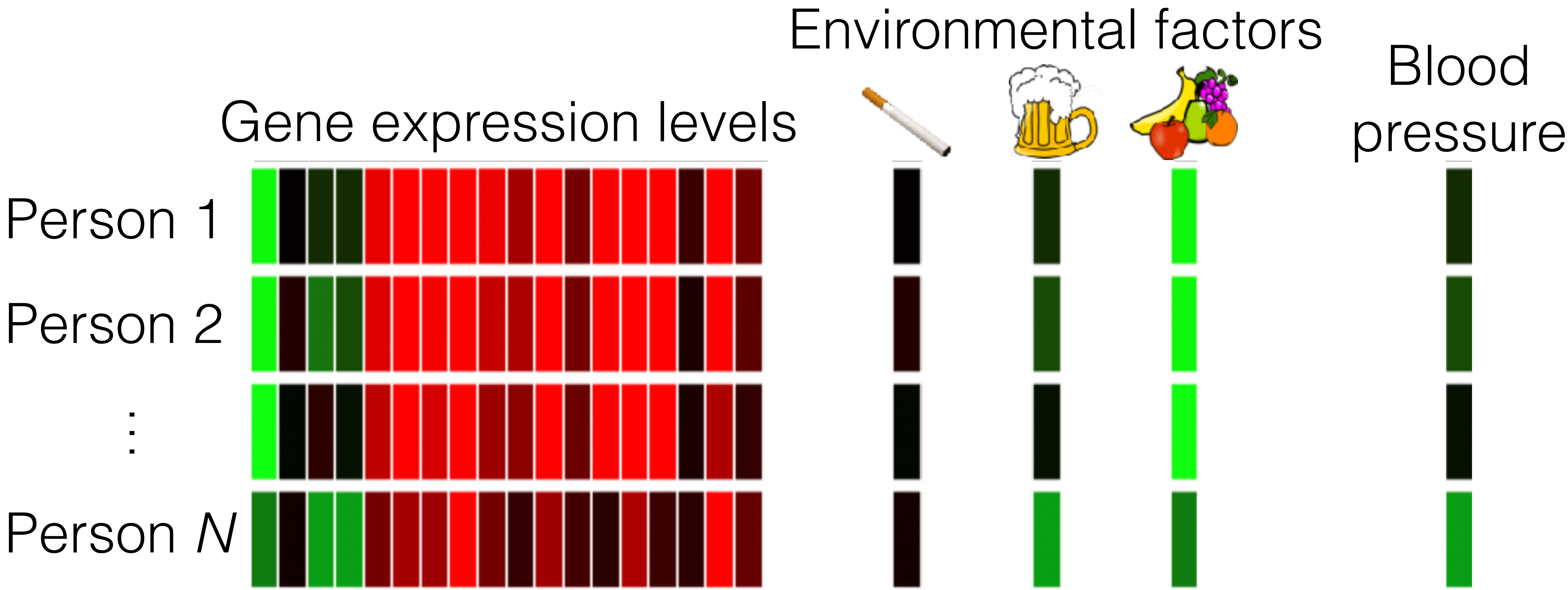

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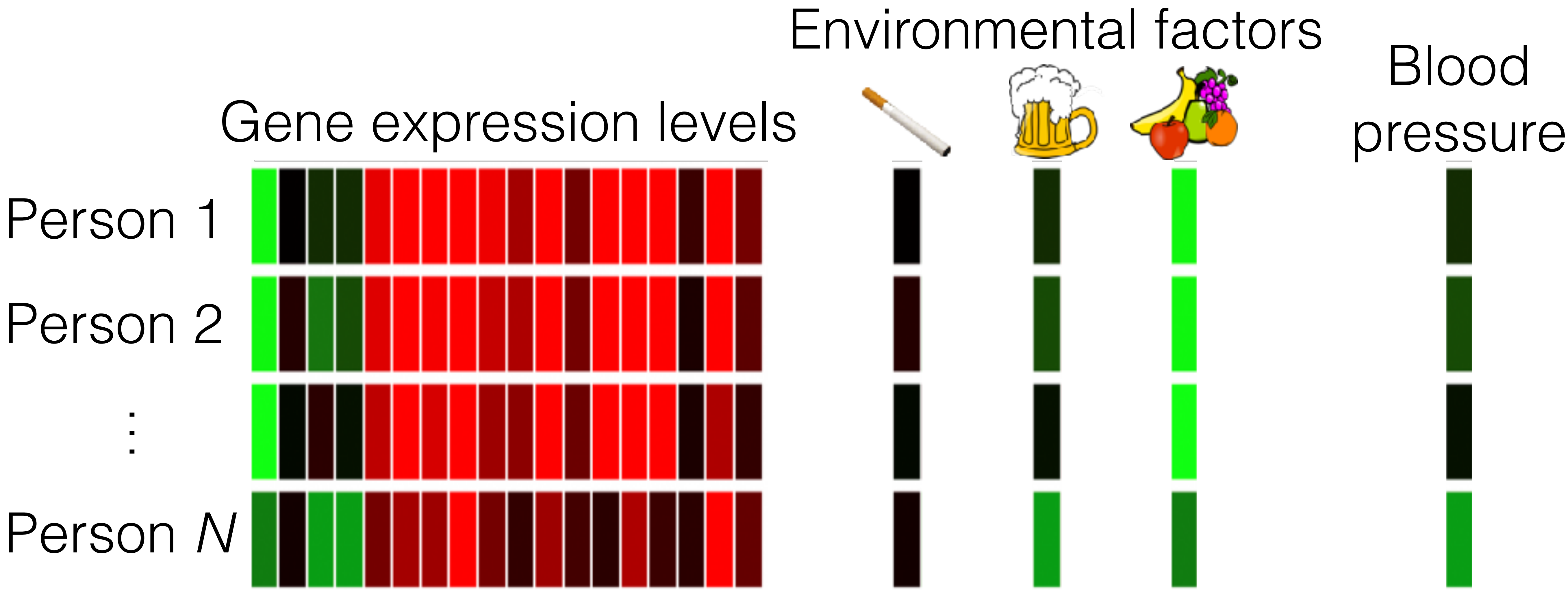
Pairwise interactions in high dimensions



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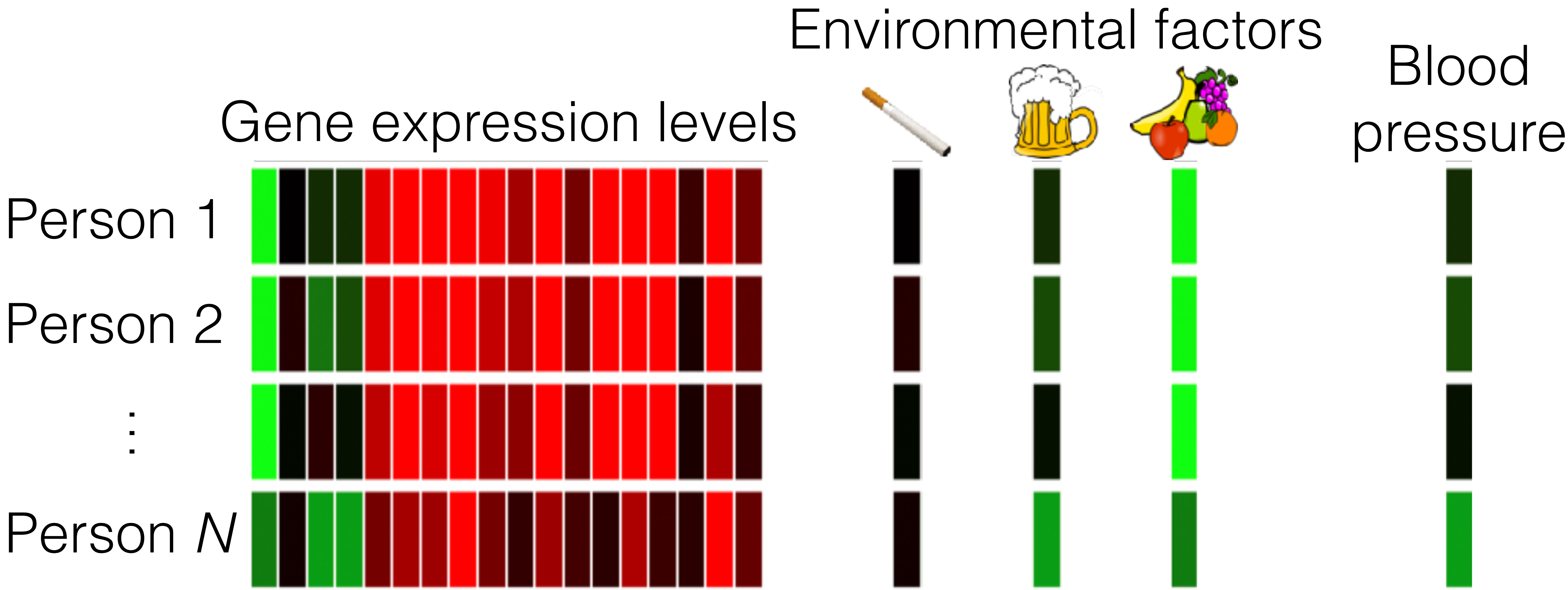

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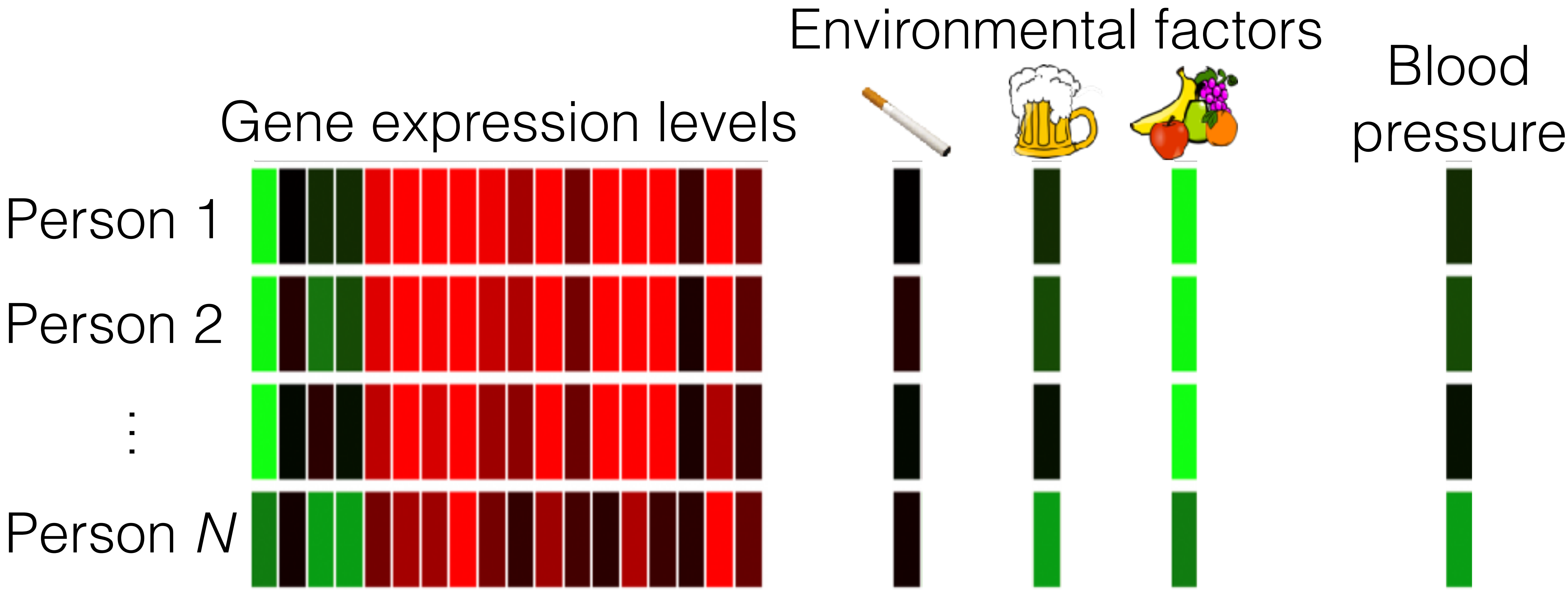

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- **We provide**: Fast, accurate (Bayes) method for interaction discovery
  - Better scaling in p & better accuracy than LASSO-based methods. Orders of magnitude faster than naive Bayesian inference

Roadmap

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- Setup: Discovering main and interaction effects

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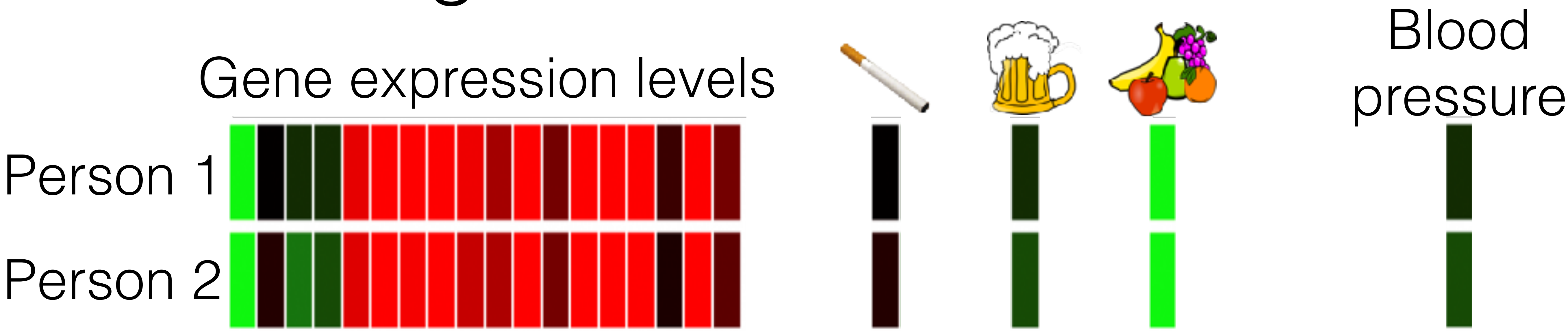
Discovering main and interaction effects



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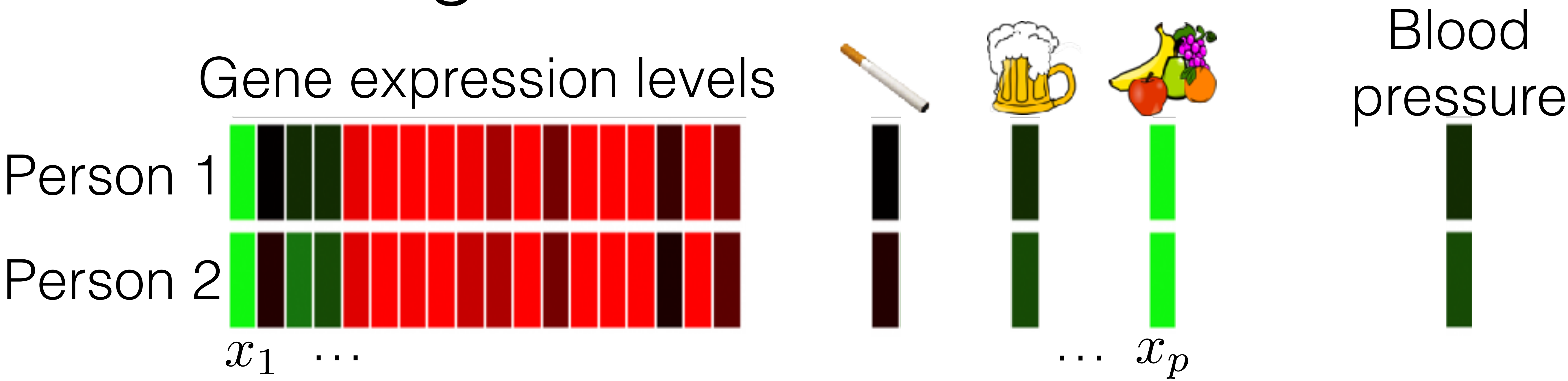

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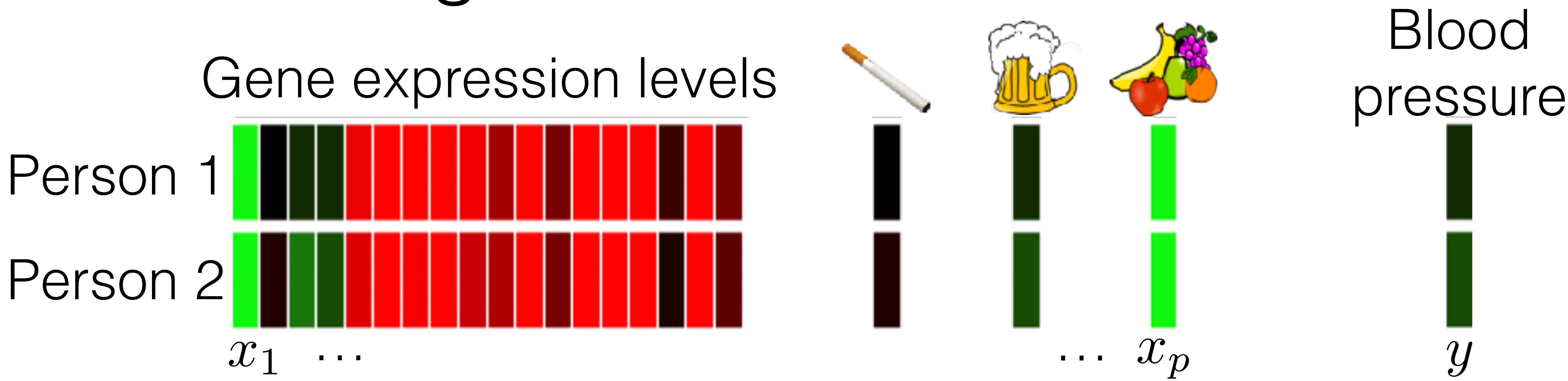

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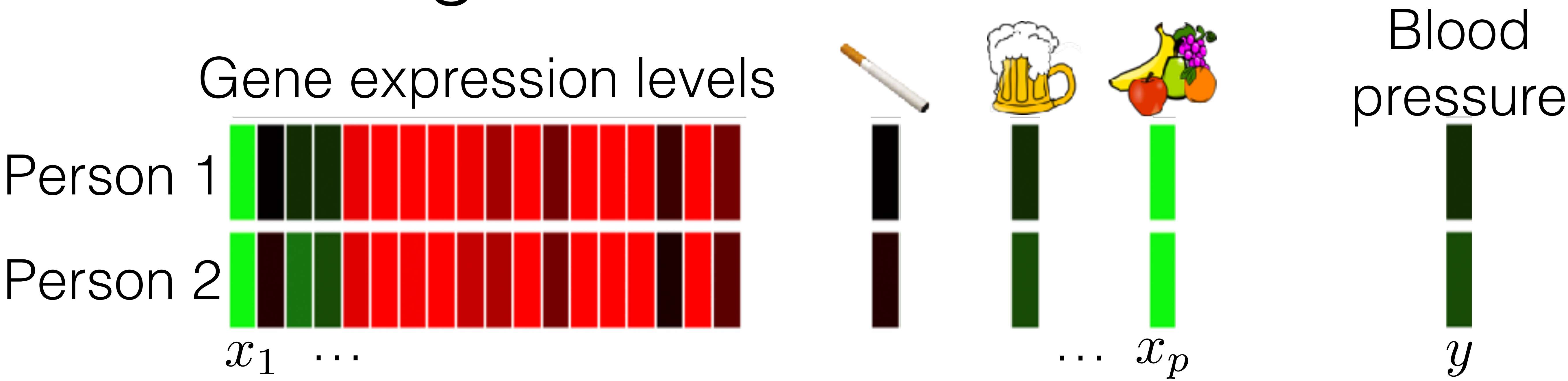

$$x^\top := [x_1, \ldots, x_p]$$

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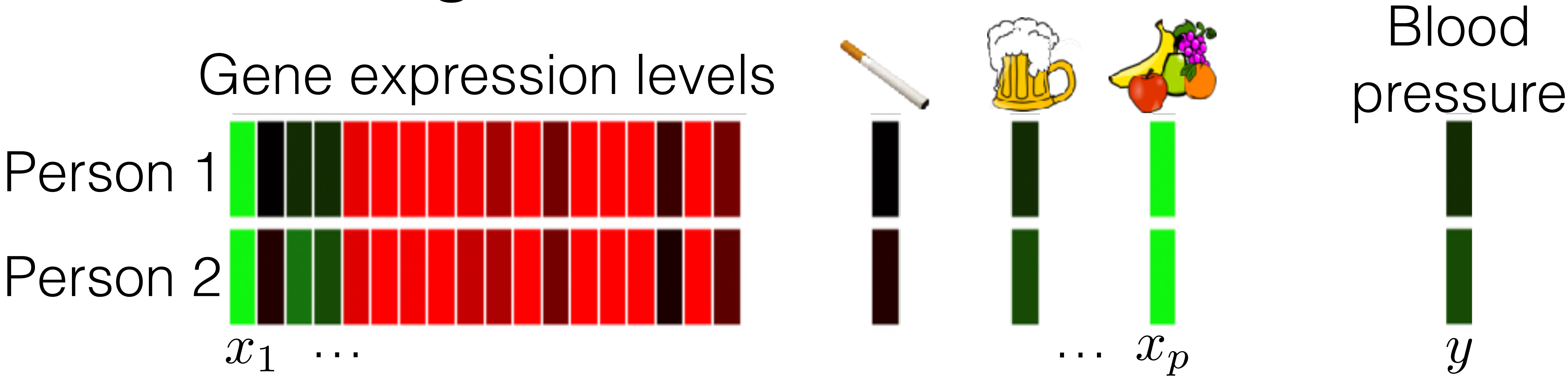

$$x^\top := [x_1, \ldots, x_p]$$

$$y^{(n)} = \theta^\top x^{(n)} + \epsilon^{(n)}, \quad \epsilon^{(n)} \overset{iid}{\sim} \mathcal{N}(0, \sigma^2)$$

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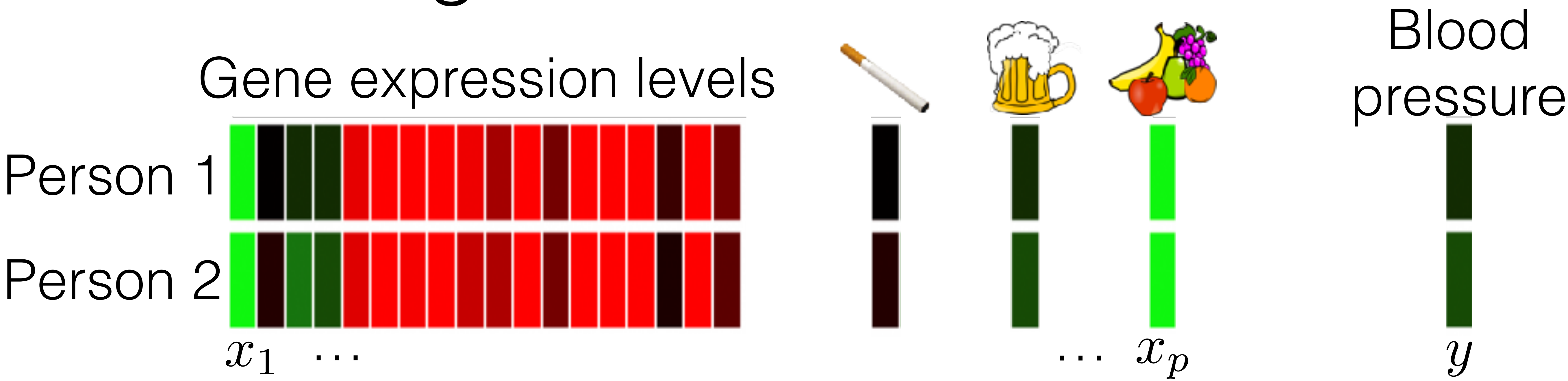

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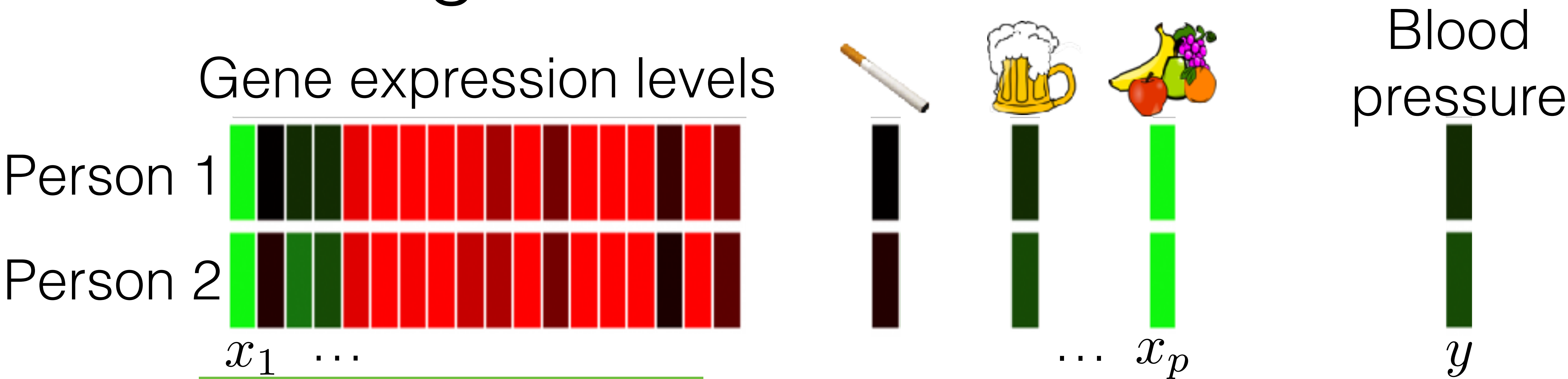

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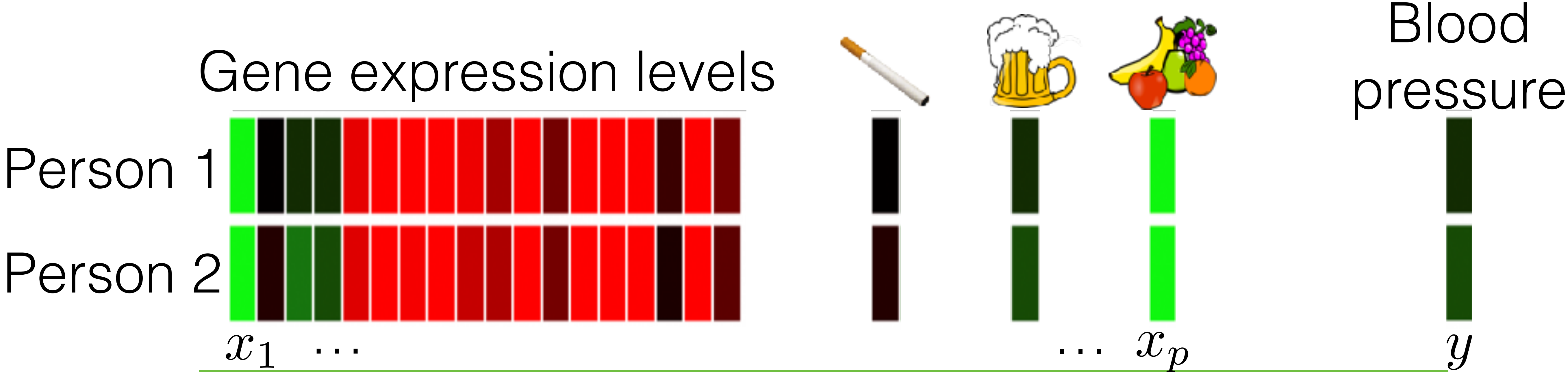

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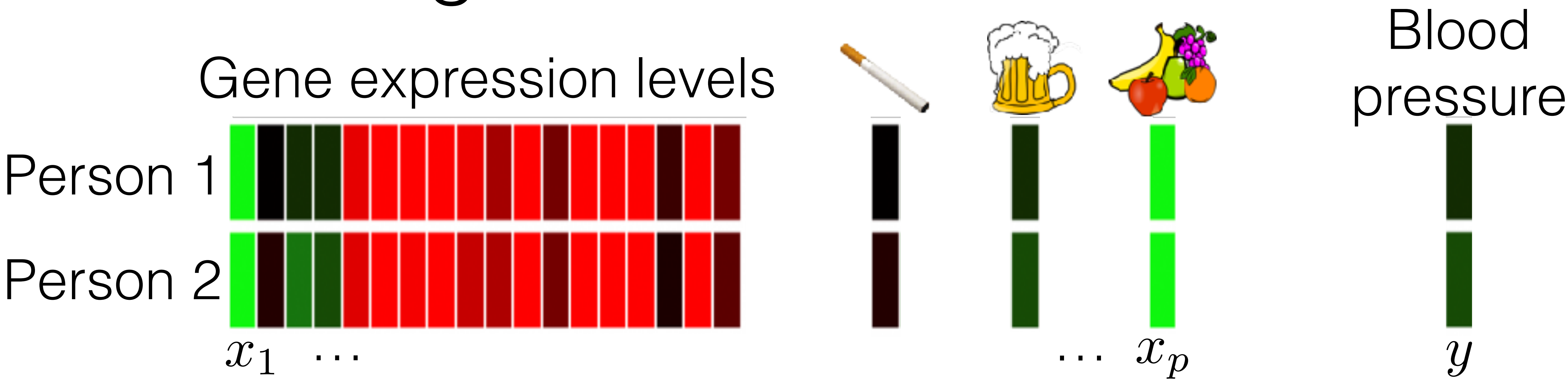

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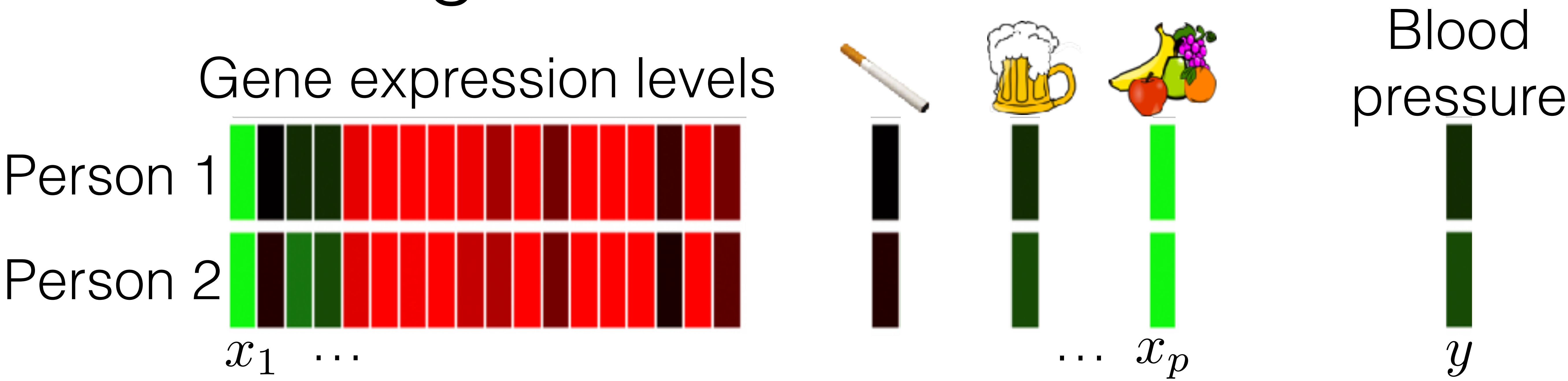

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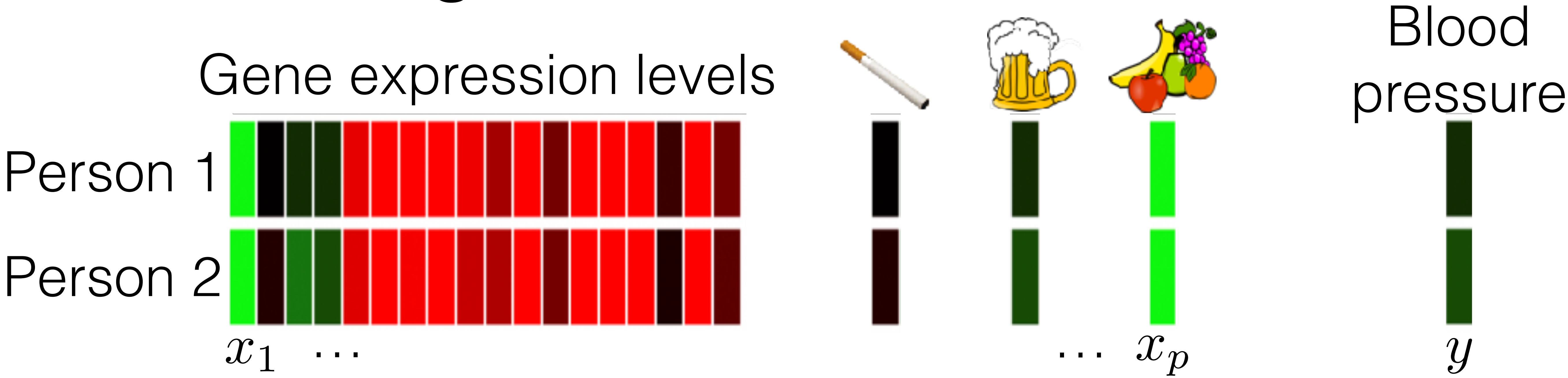

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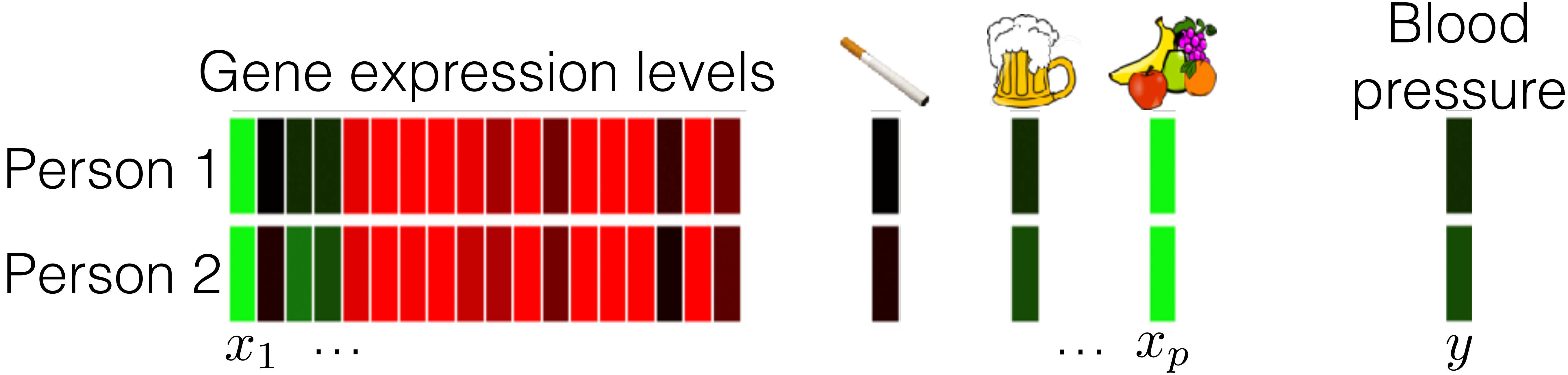

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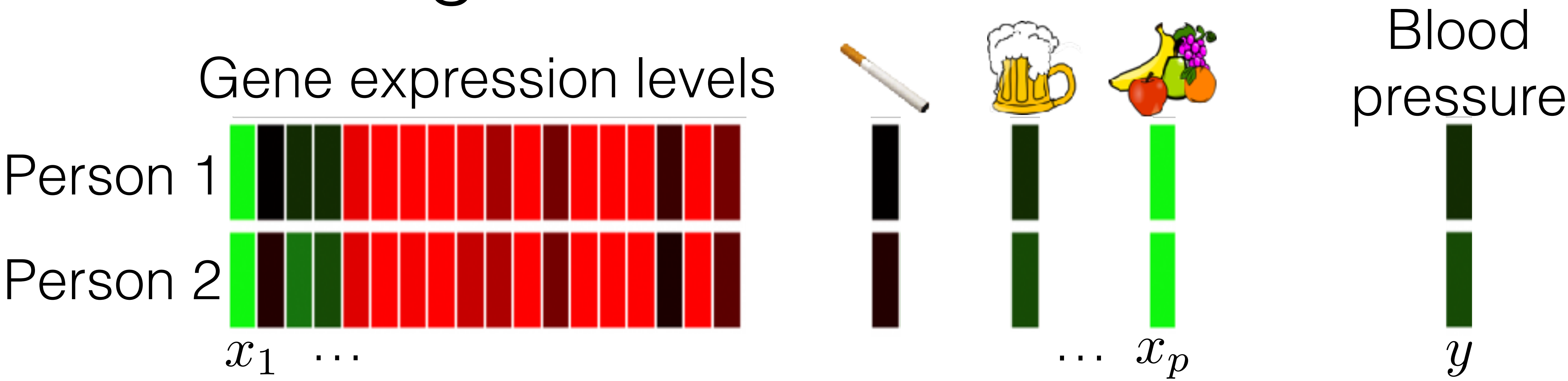

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- **Goal**: Parameter selection/estimation under assumptions:

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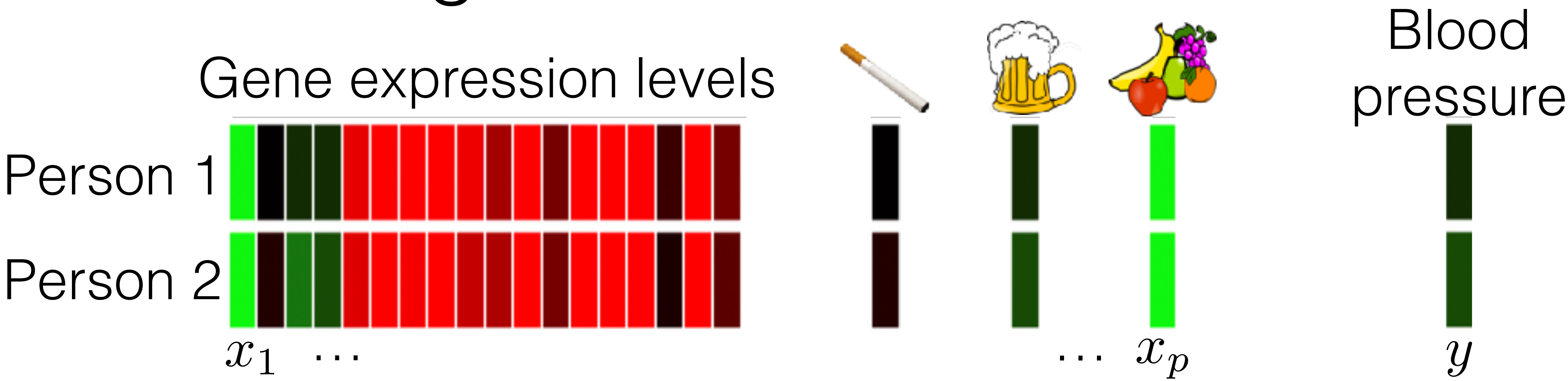

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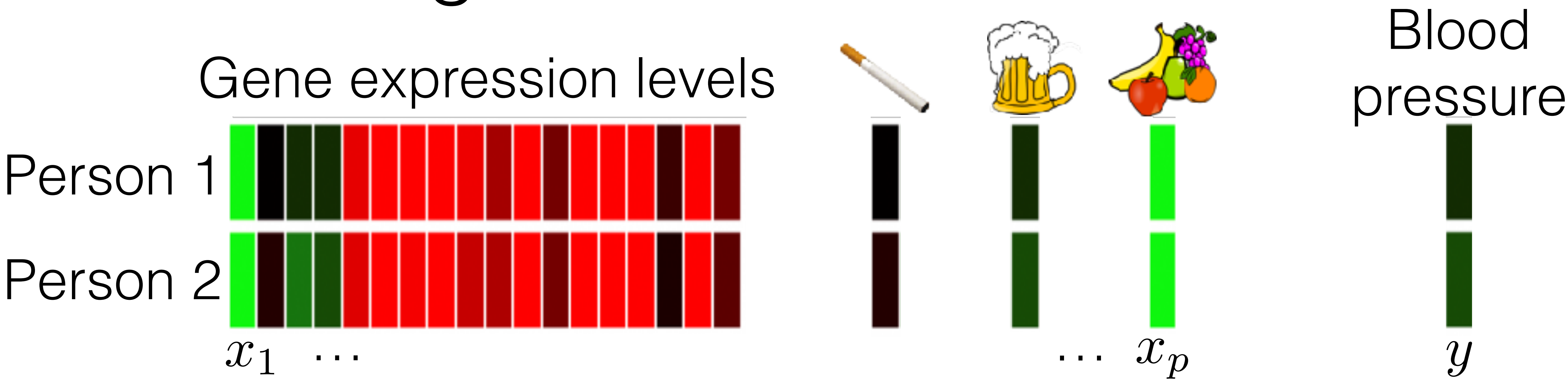

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[Chipman 1996; Wu et al 2009; Bien et al 2013; Lim, Hastie 2015; Nakagawa et al 2016; Griffin, Brown 2017]

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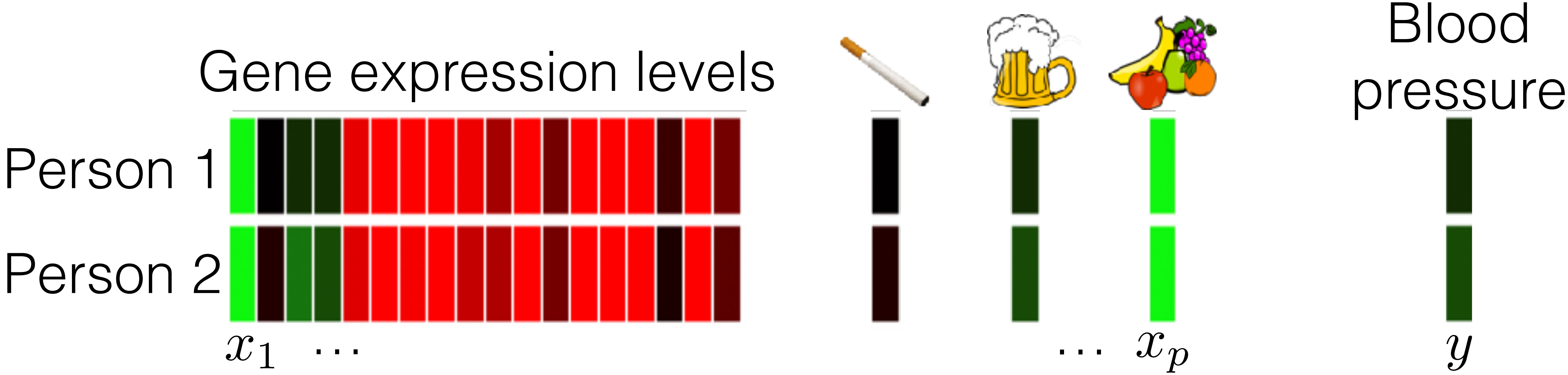

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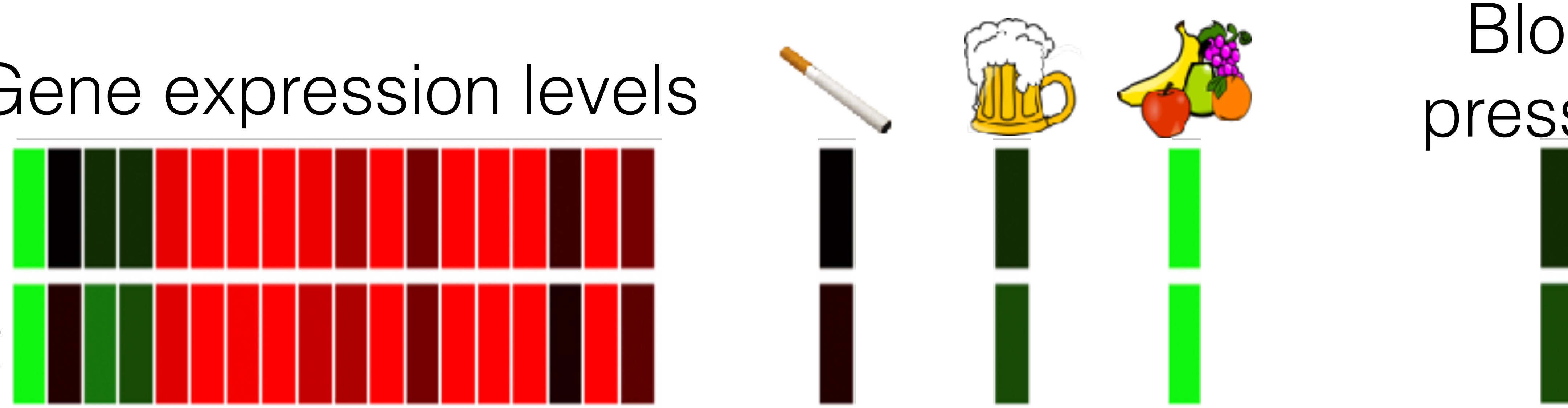

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- **Our solution**: using structure in covariates + sparsity assumptions to reduce to a problem *linear* in p

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Not just for SKIM

Kernel Interaction Sampler vs. Naive MCMC

- MCMC option 1: sample θ

Kernel Interaction Sampler vs. Naive MCMC

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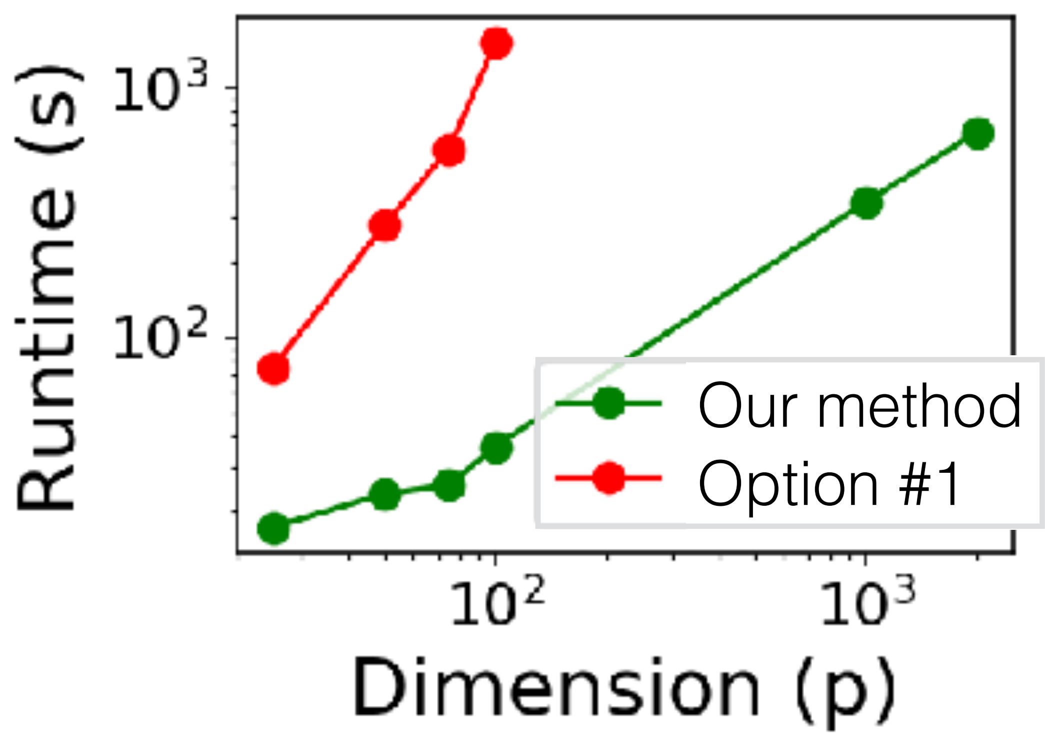

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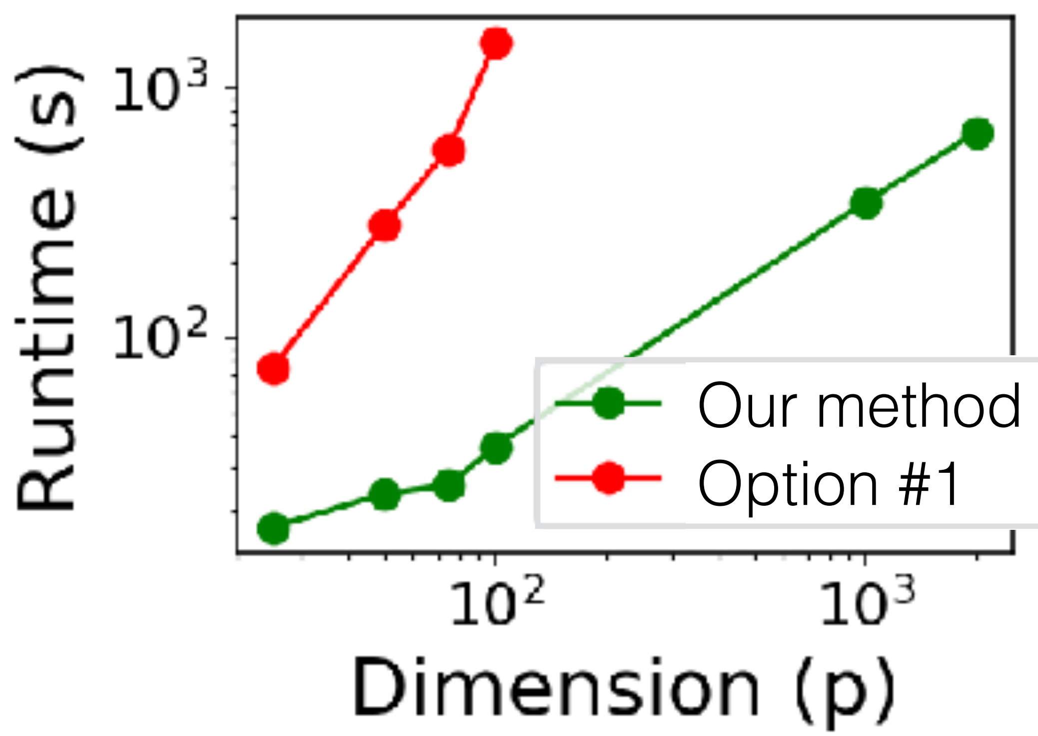

- Mixing (1000 iters Stan):
  - Option #1: all $\hat{R} > 1.05$
  - Our method: all $\hat{R} < 1.05$

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- MCMC option 2: use conditional conjugacy for θ

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$$X^\top X$$

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$$X^\top X \quad + \quad \text{prior precision matrix}$$

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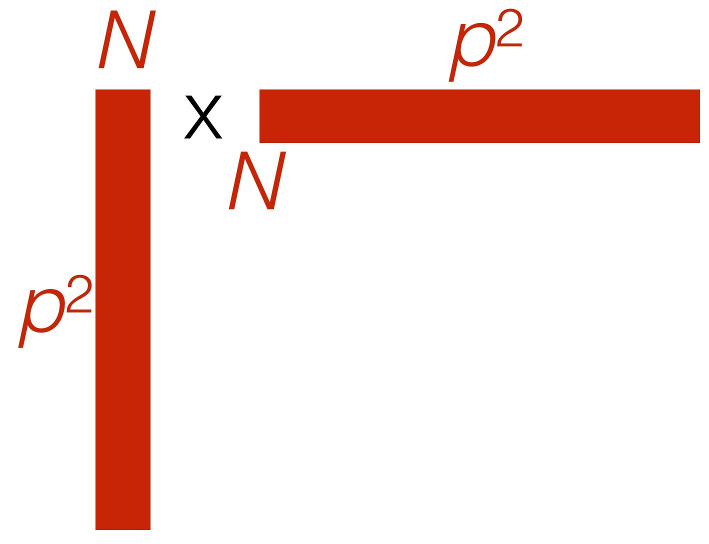

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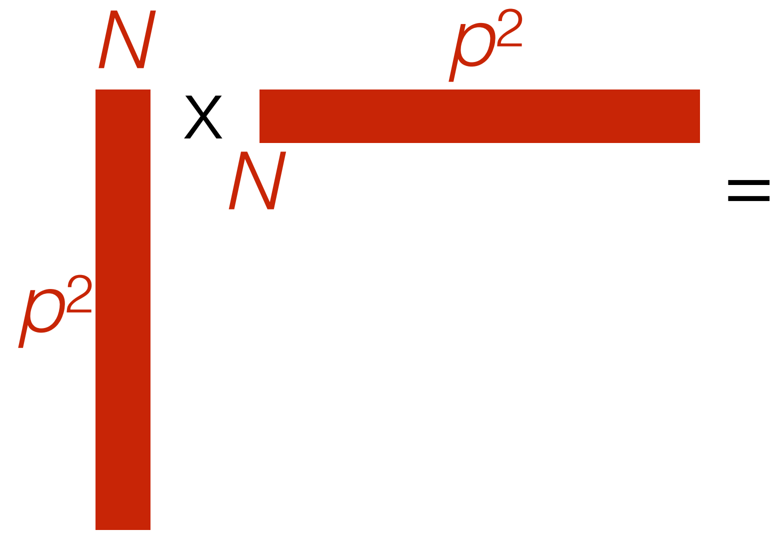

Kernel Interaction Sampler vs. Naive MCMC

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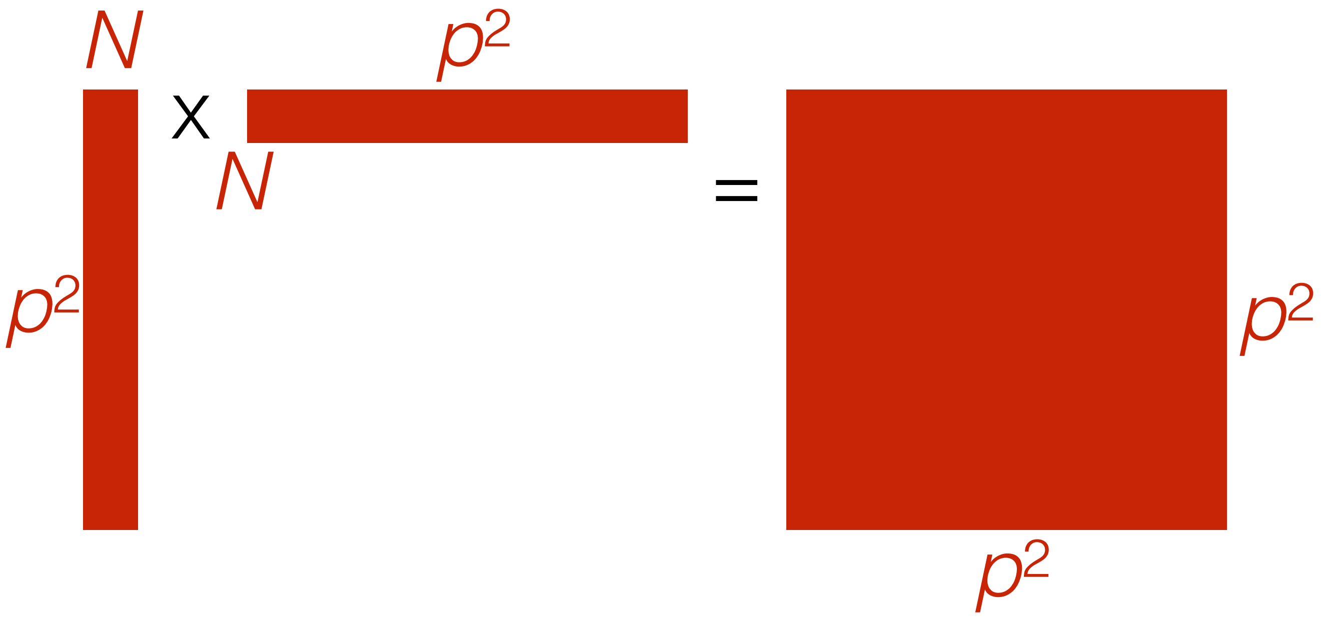

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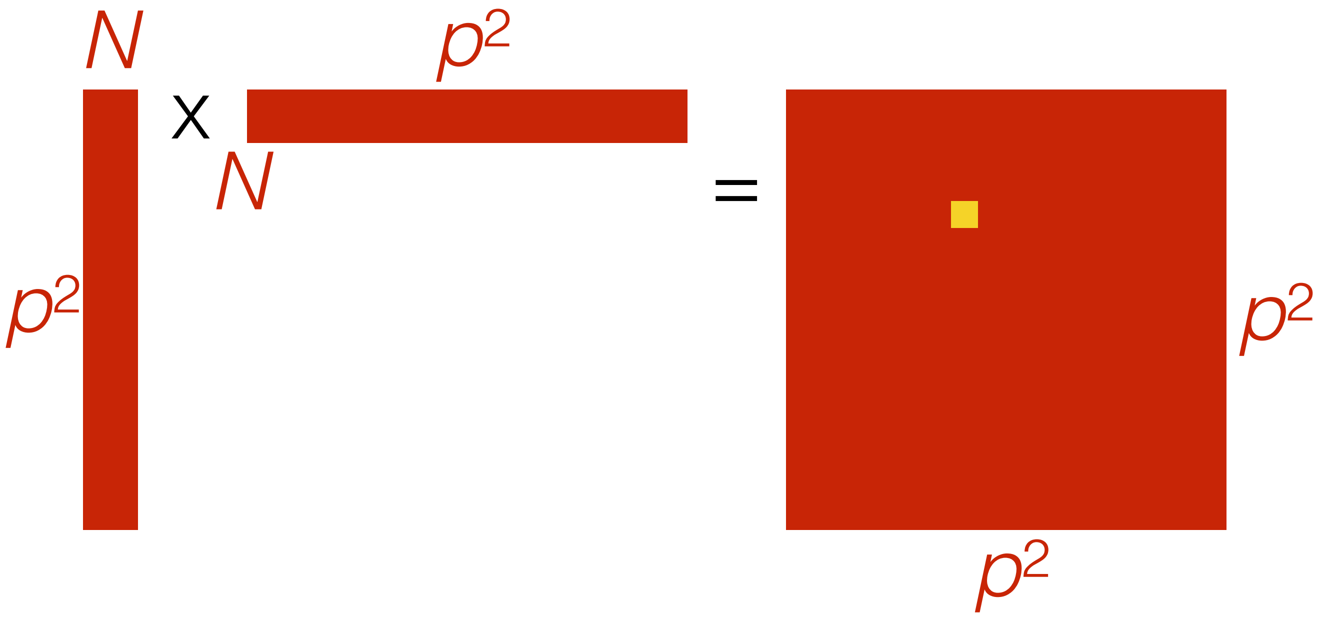

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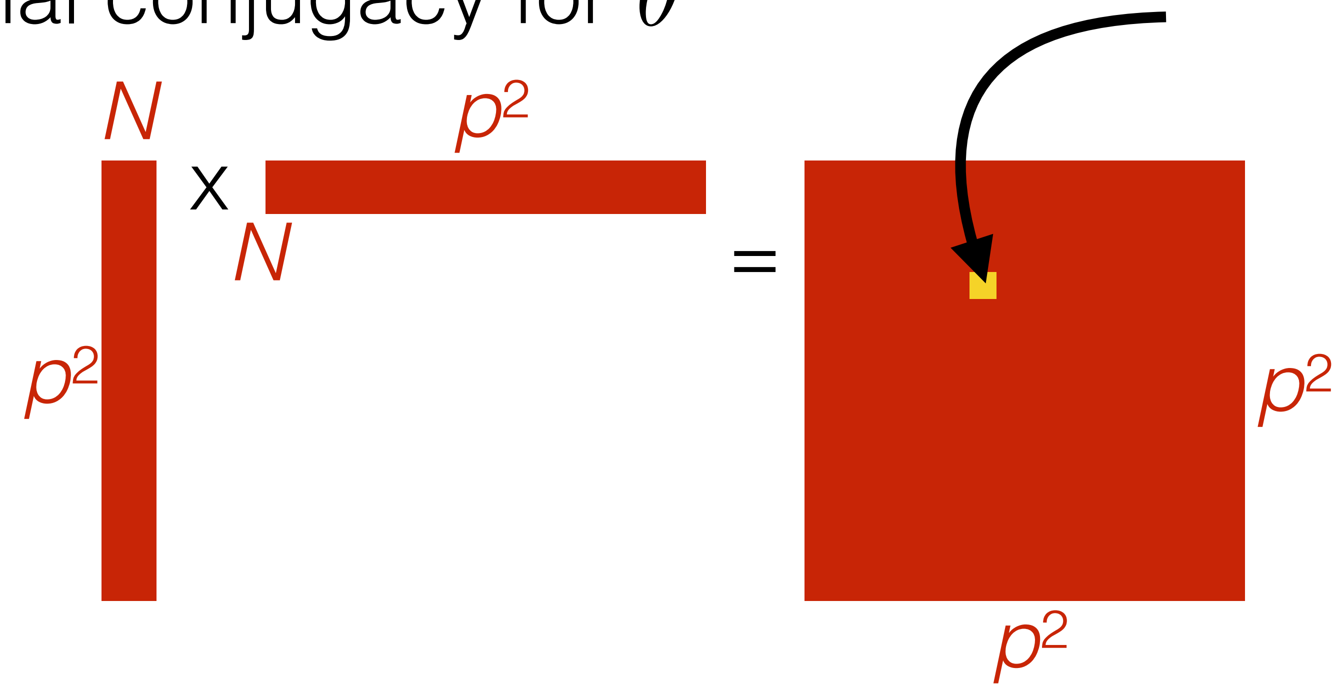

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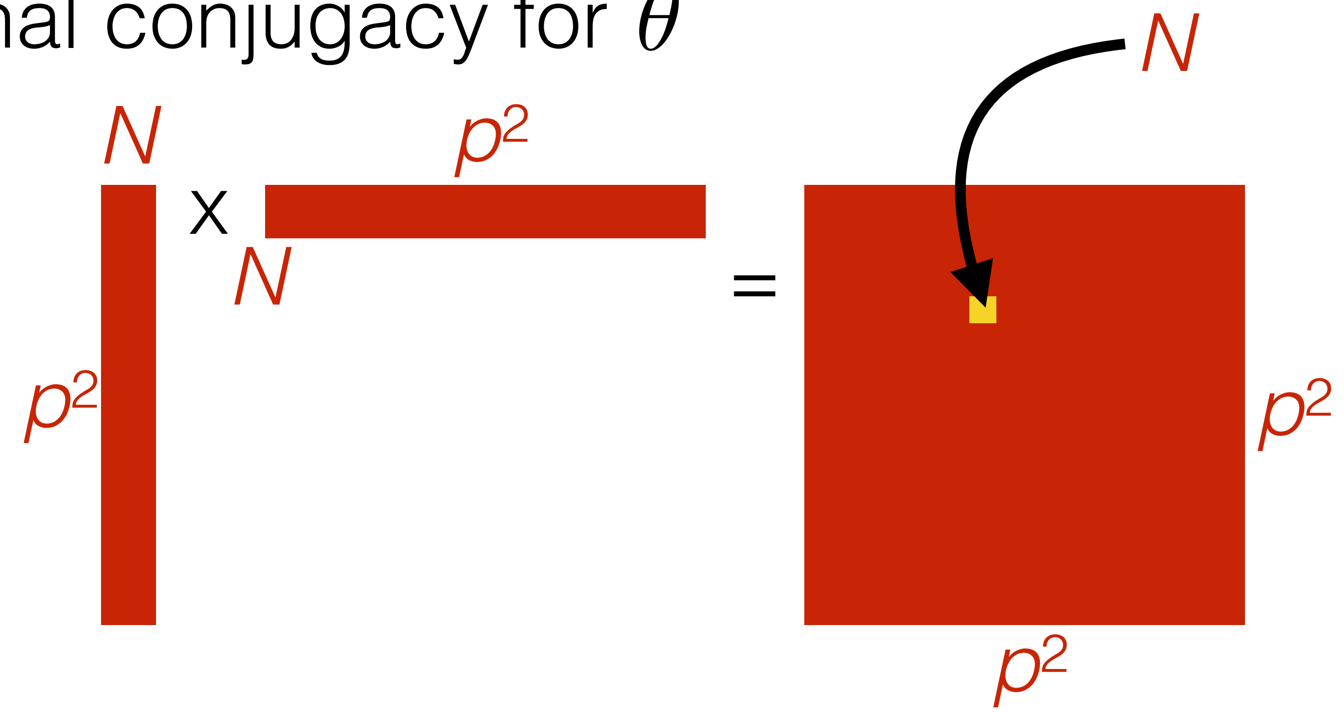

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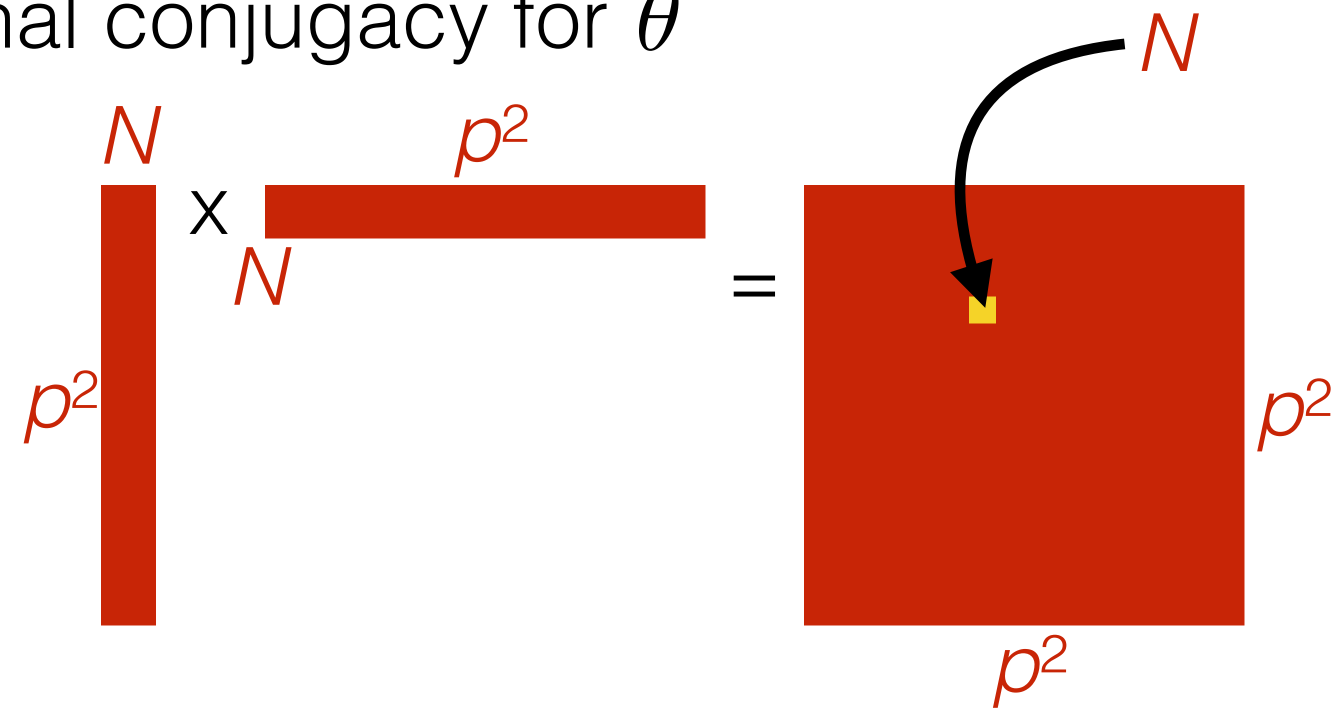

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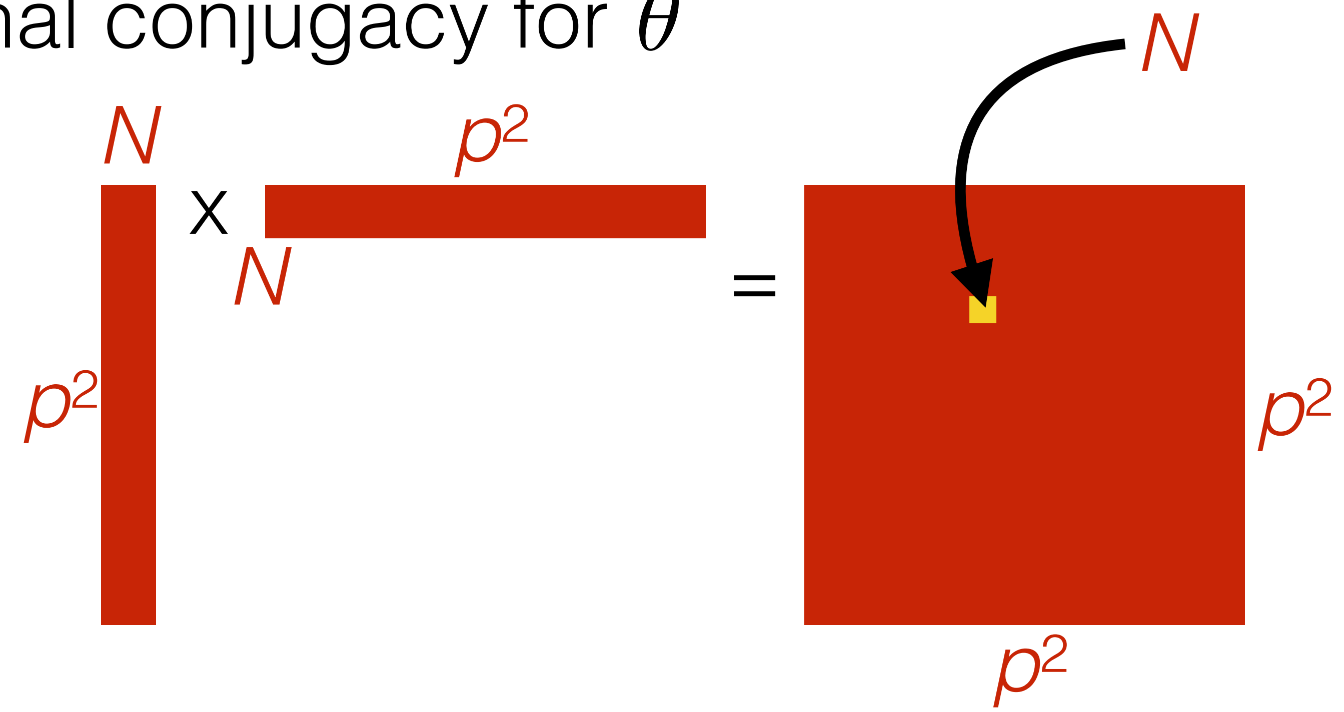

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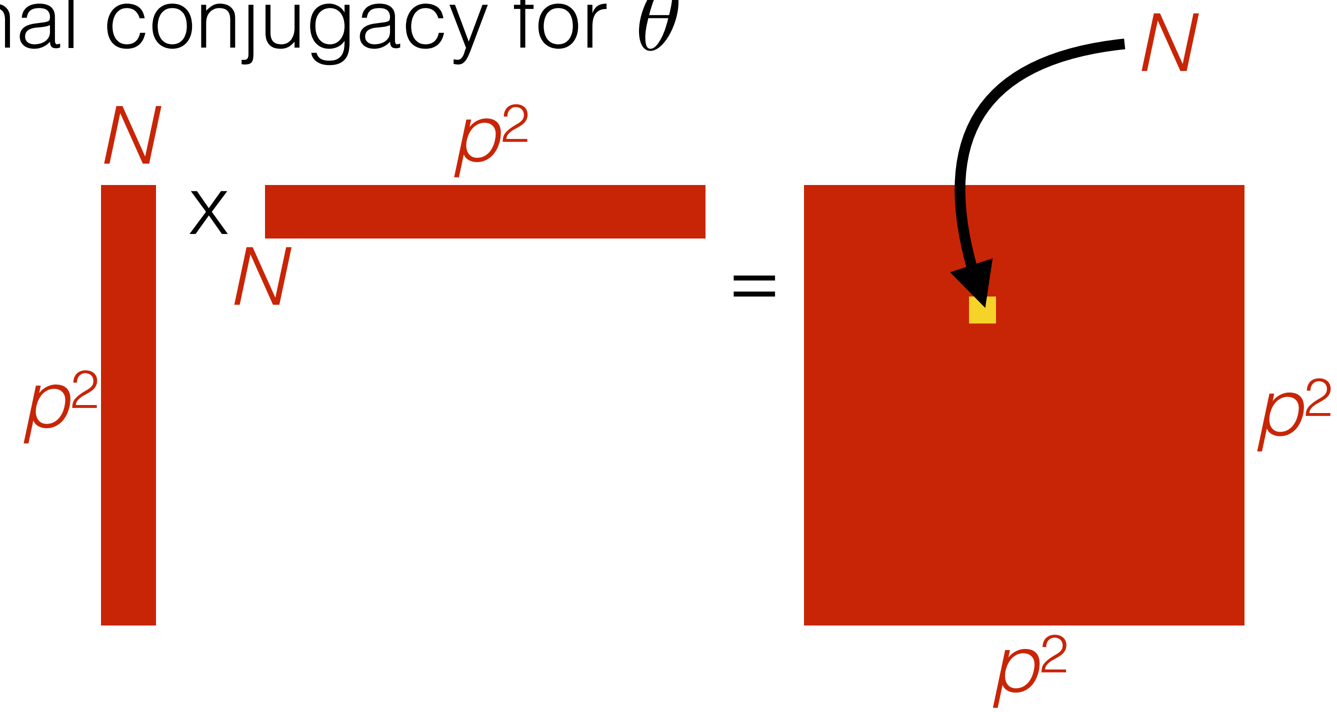

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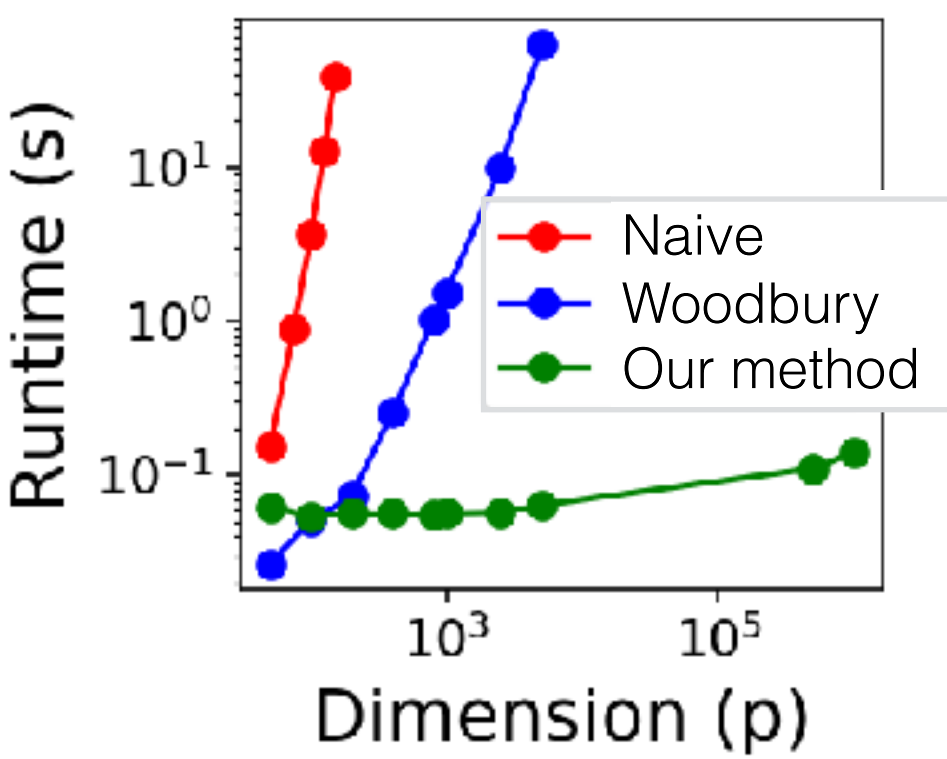

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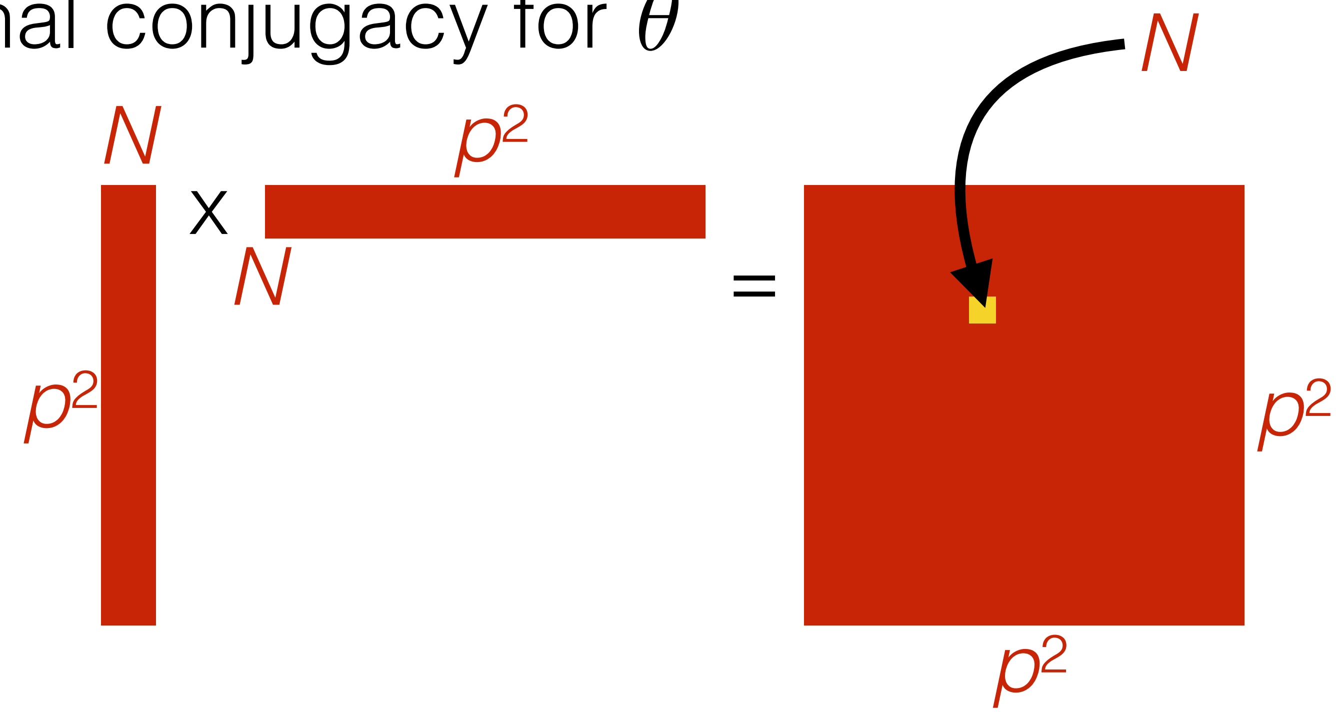

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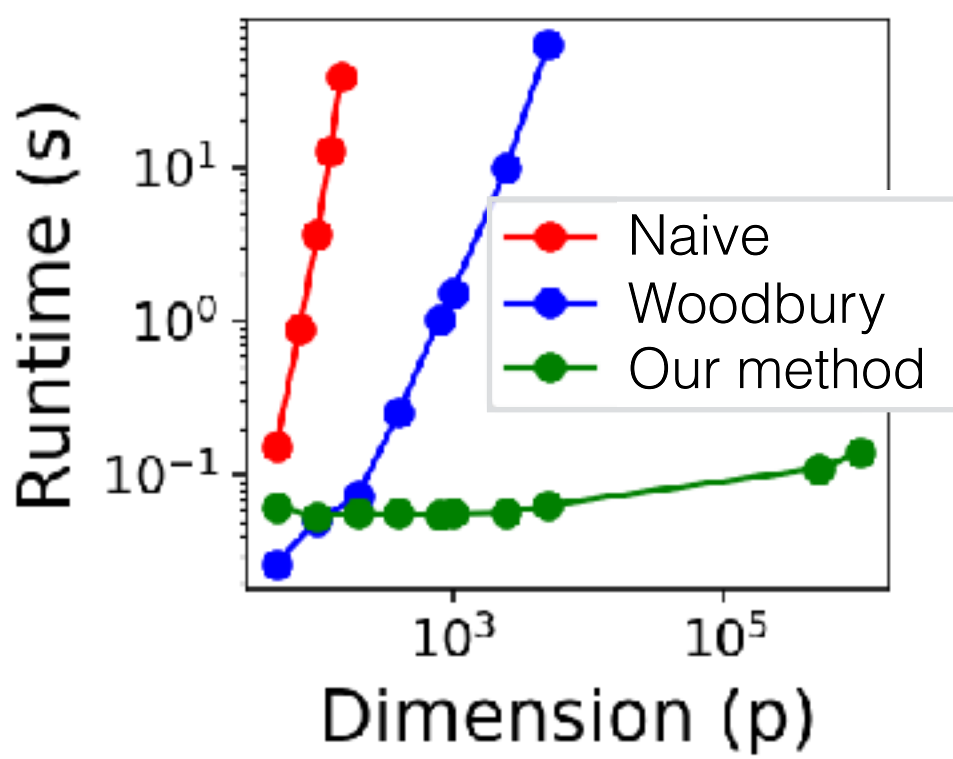

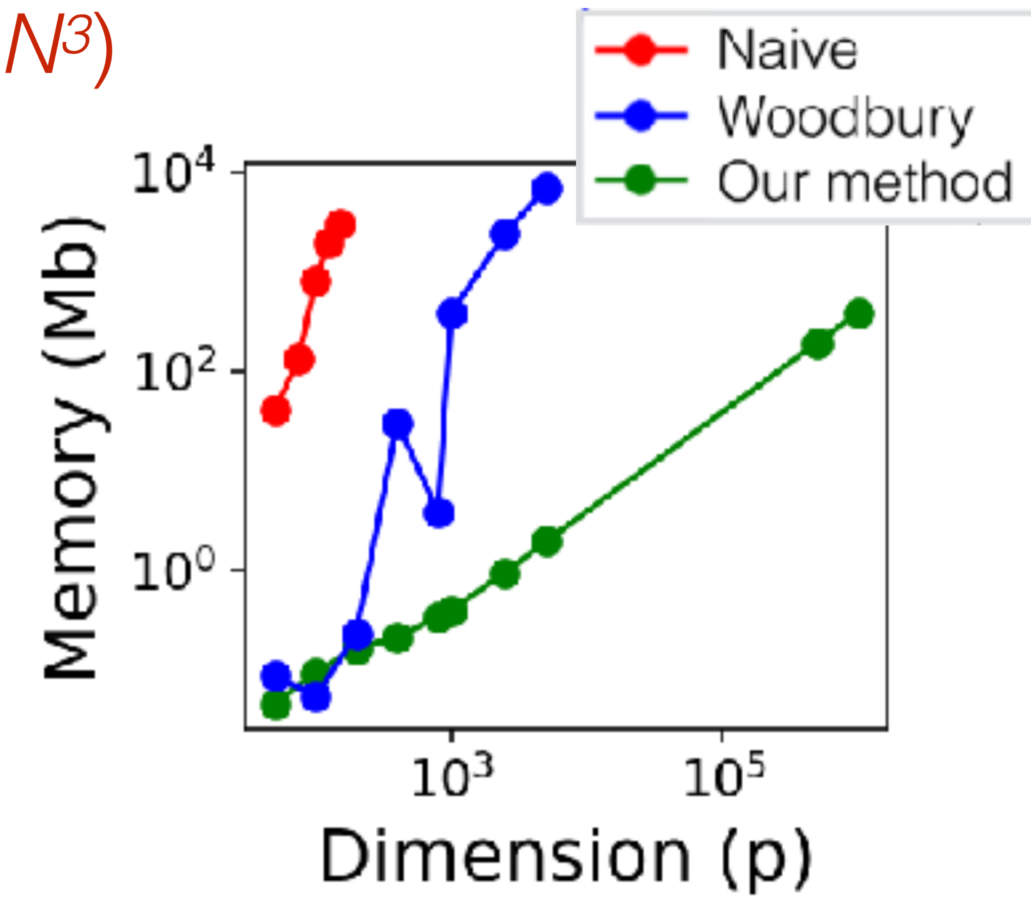

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Kernel Interaction Sampler vs. Naive MCMC

use conditional conjugacy for $\theta^T \Phi_2(X)$

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Kernel Interaction Sampler vs. Naive MCMC

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X: *N*×*p*

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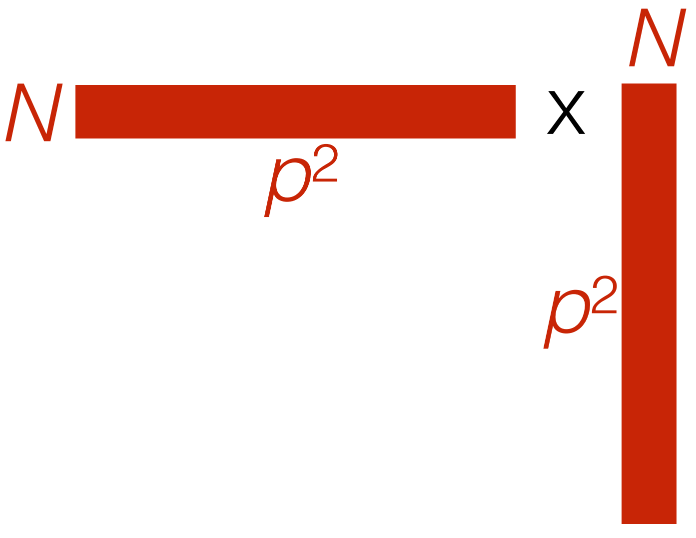

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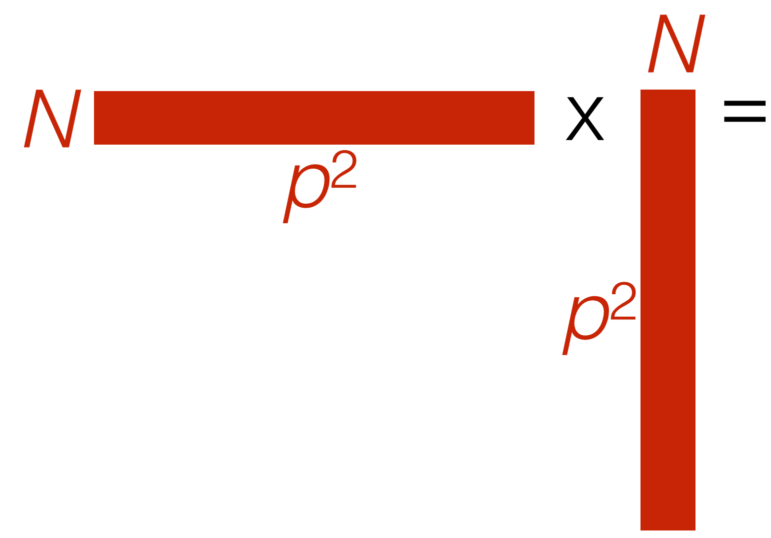

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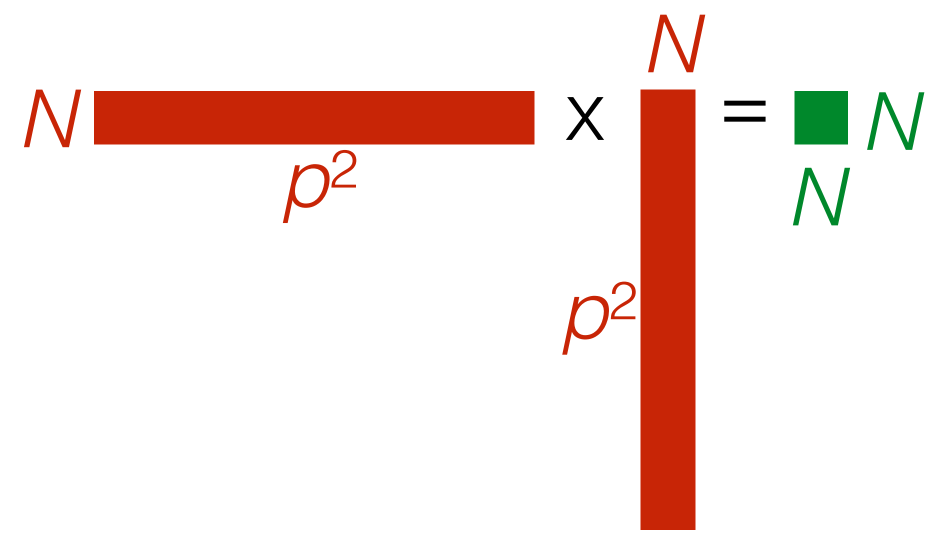

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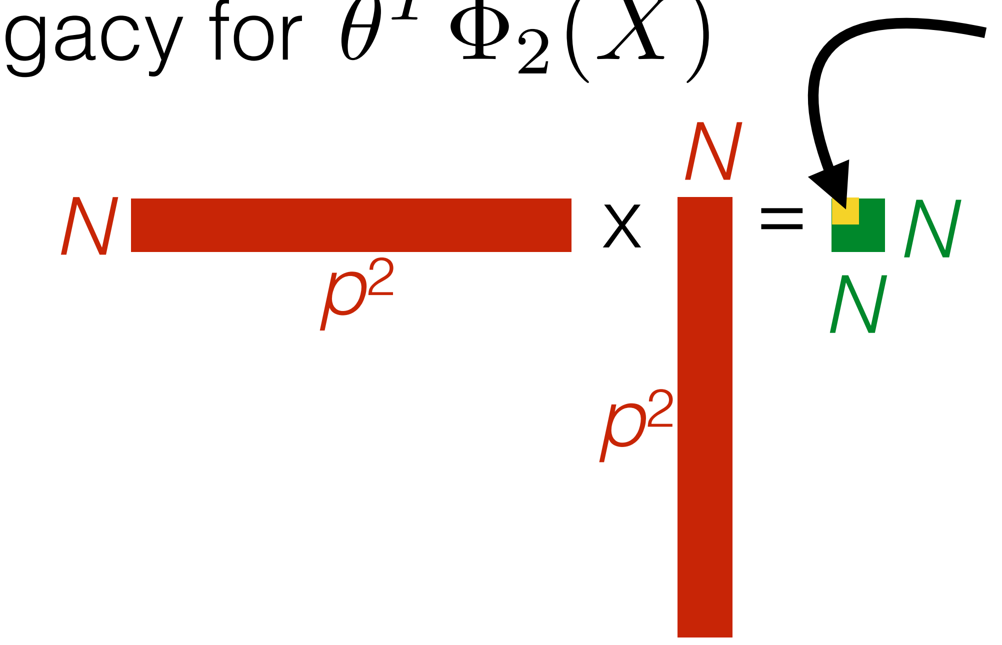

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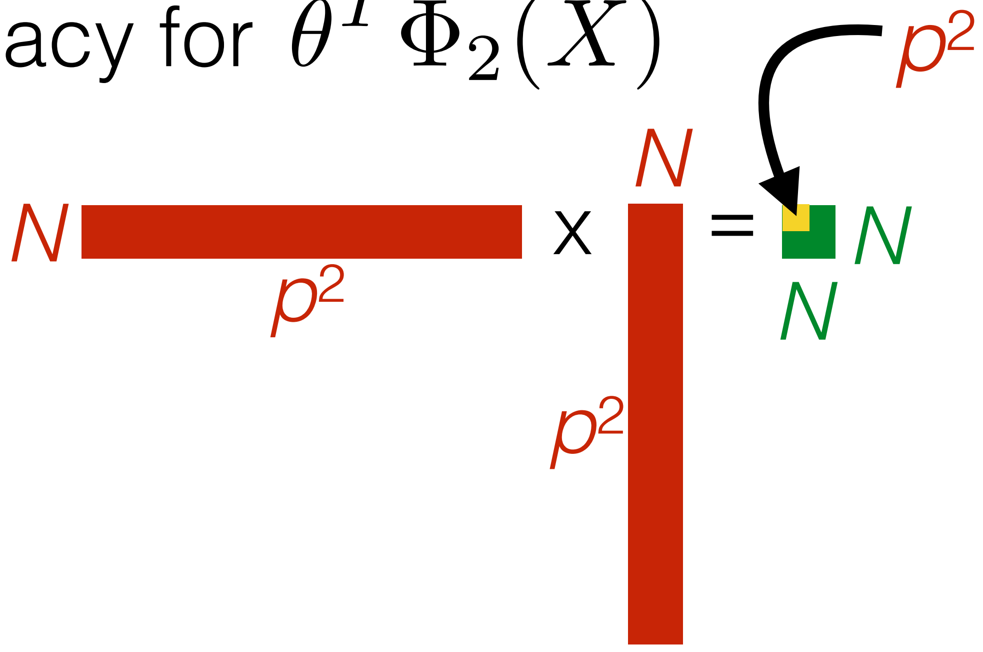

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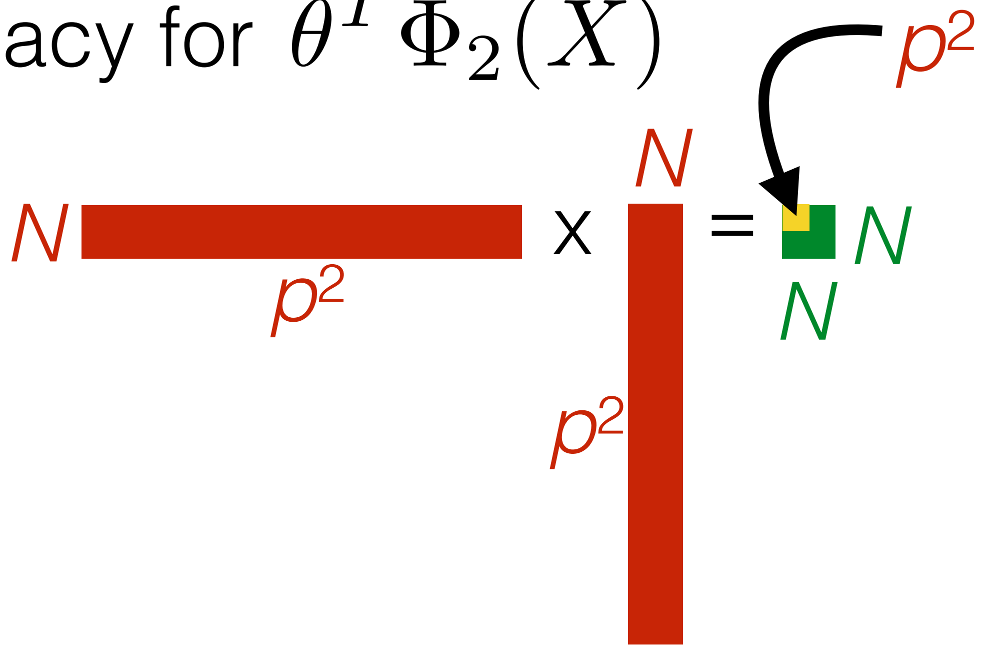

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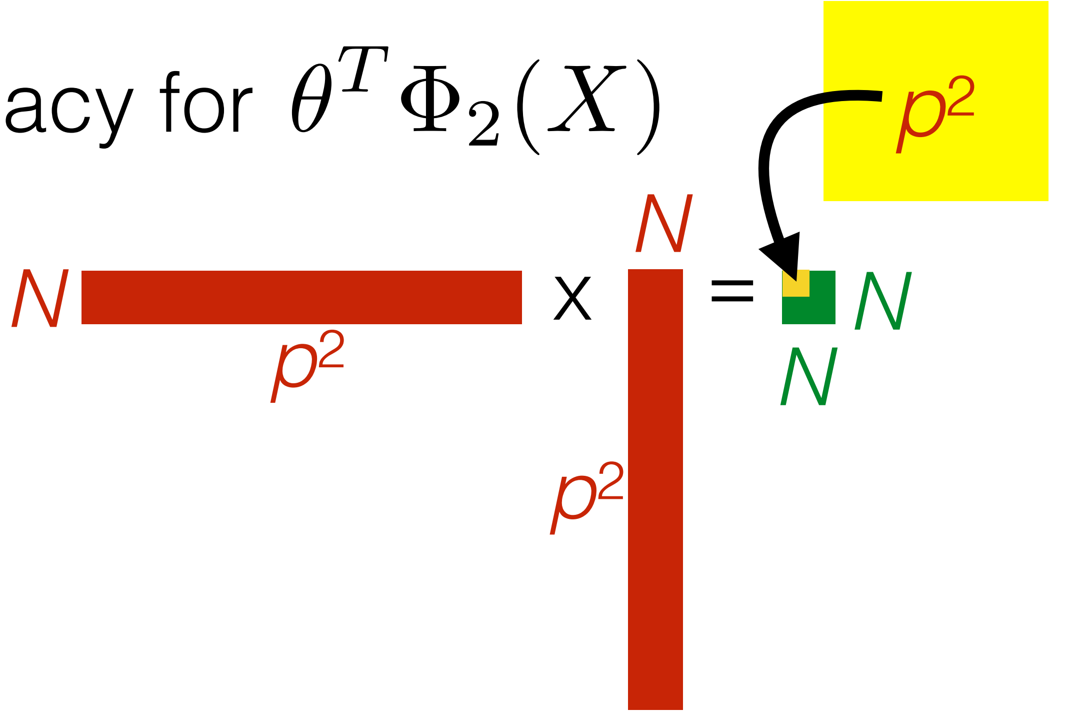

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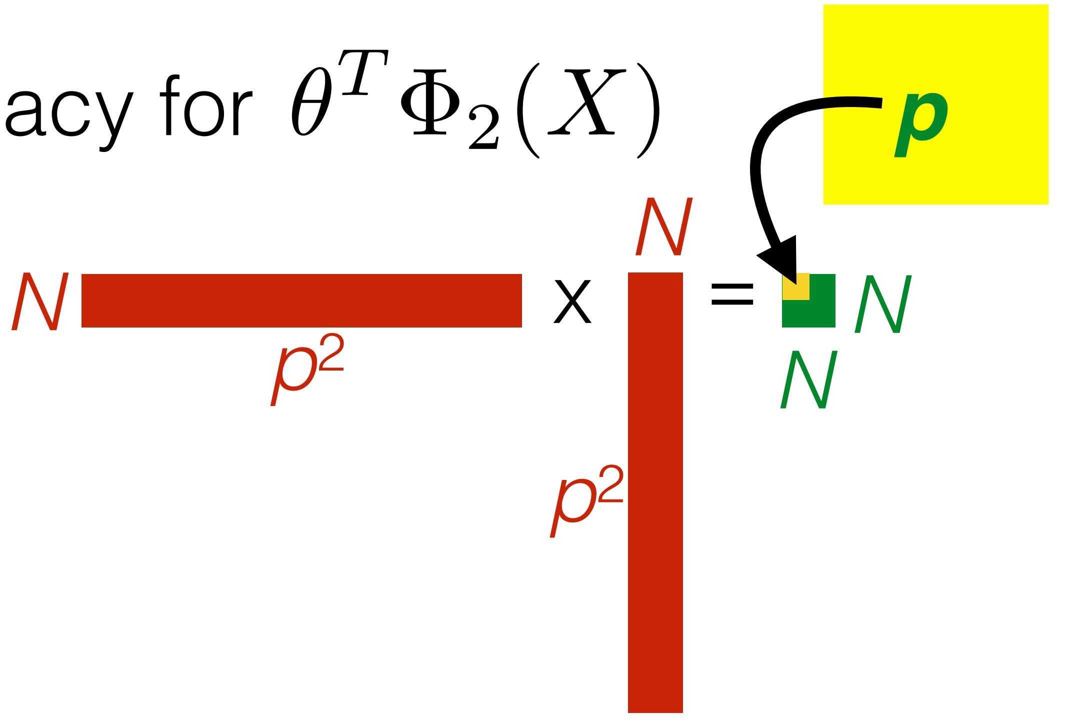

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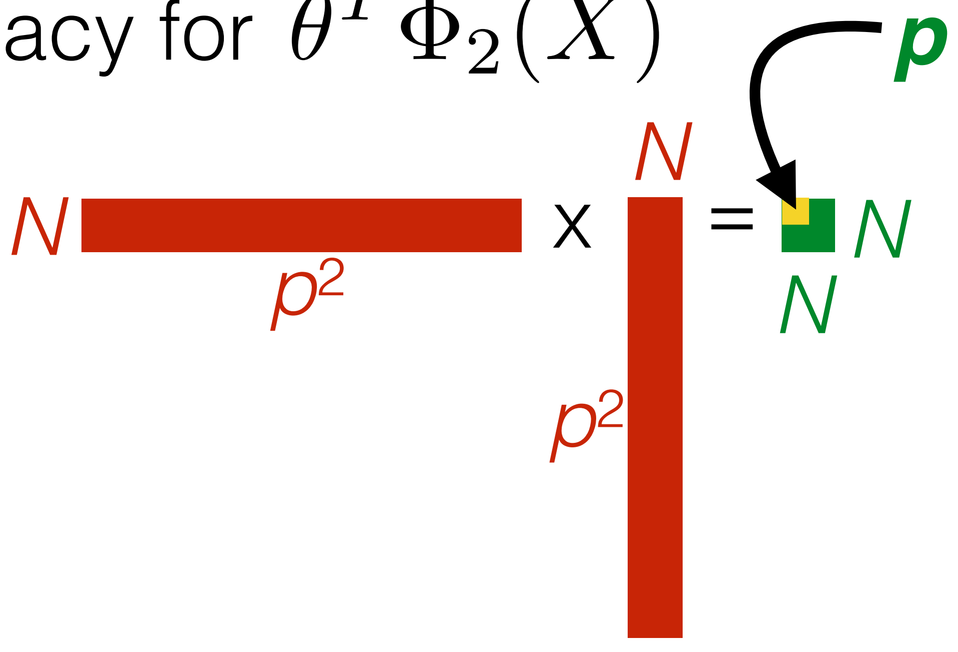

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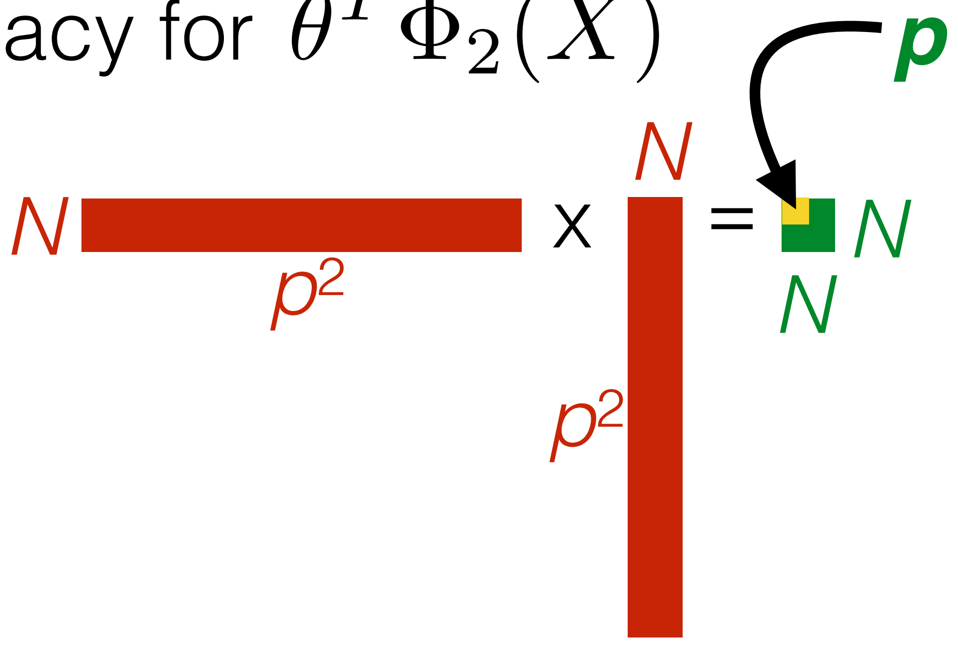

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  - A Bayesian generative model
  - Fast inference
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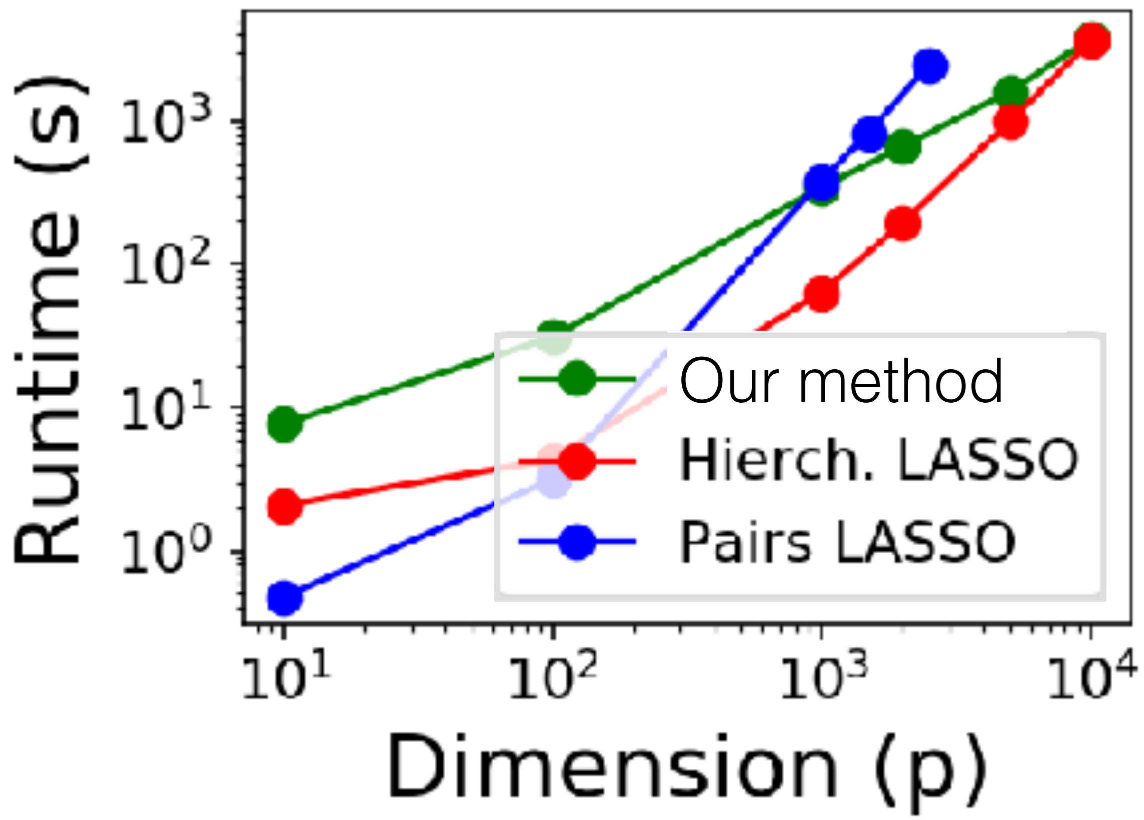

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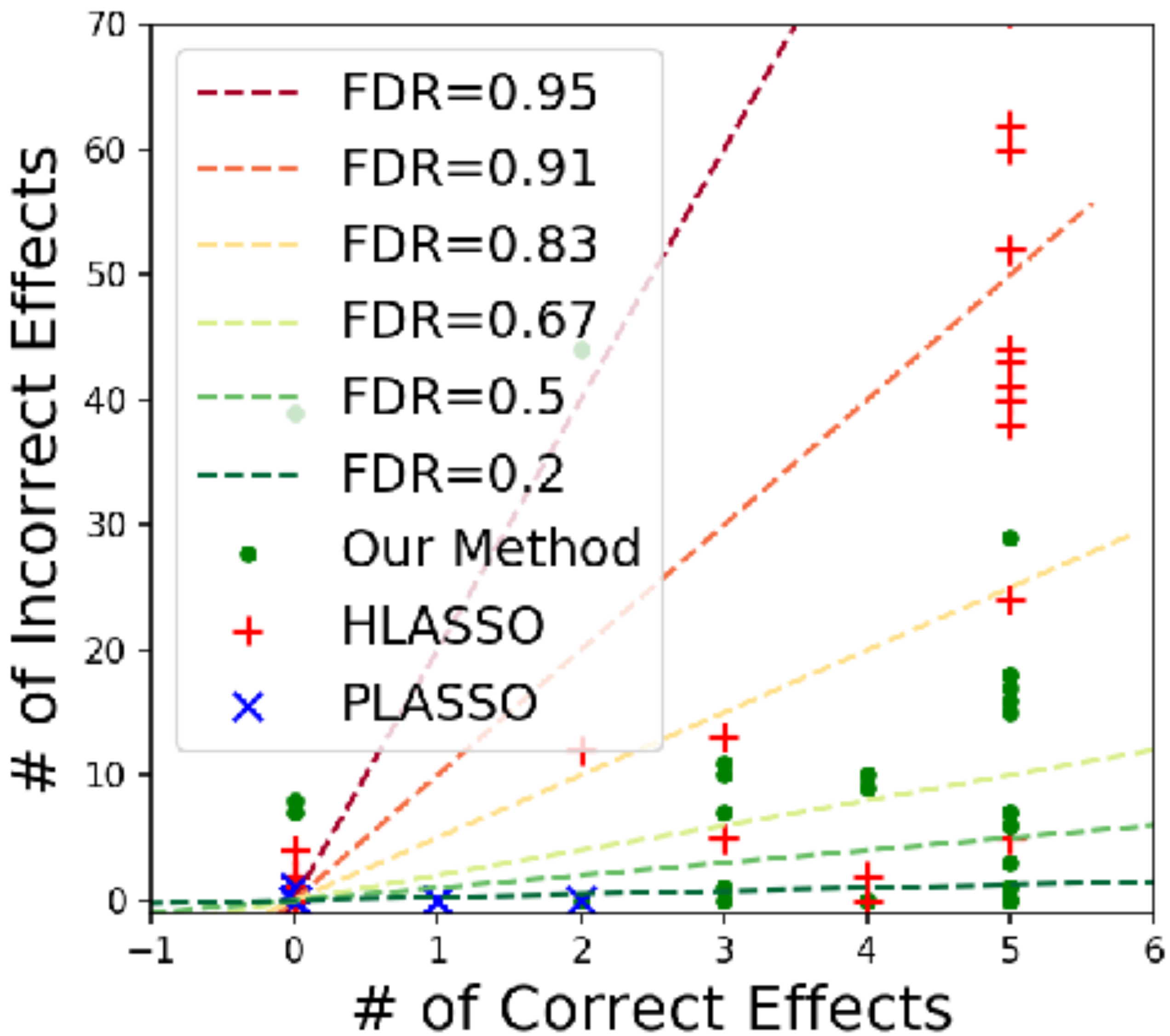
Main effects



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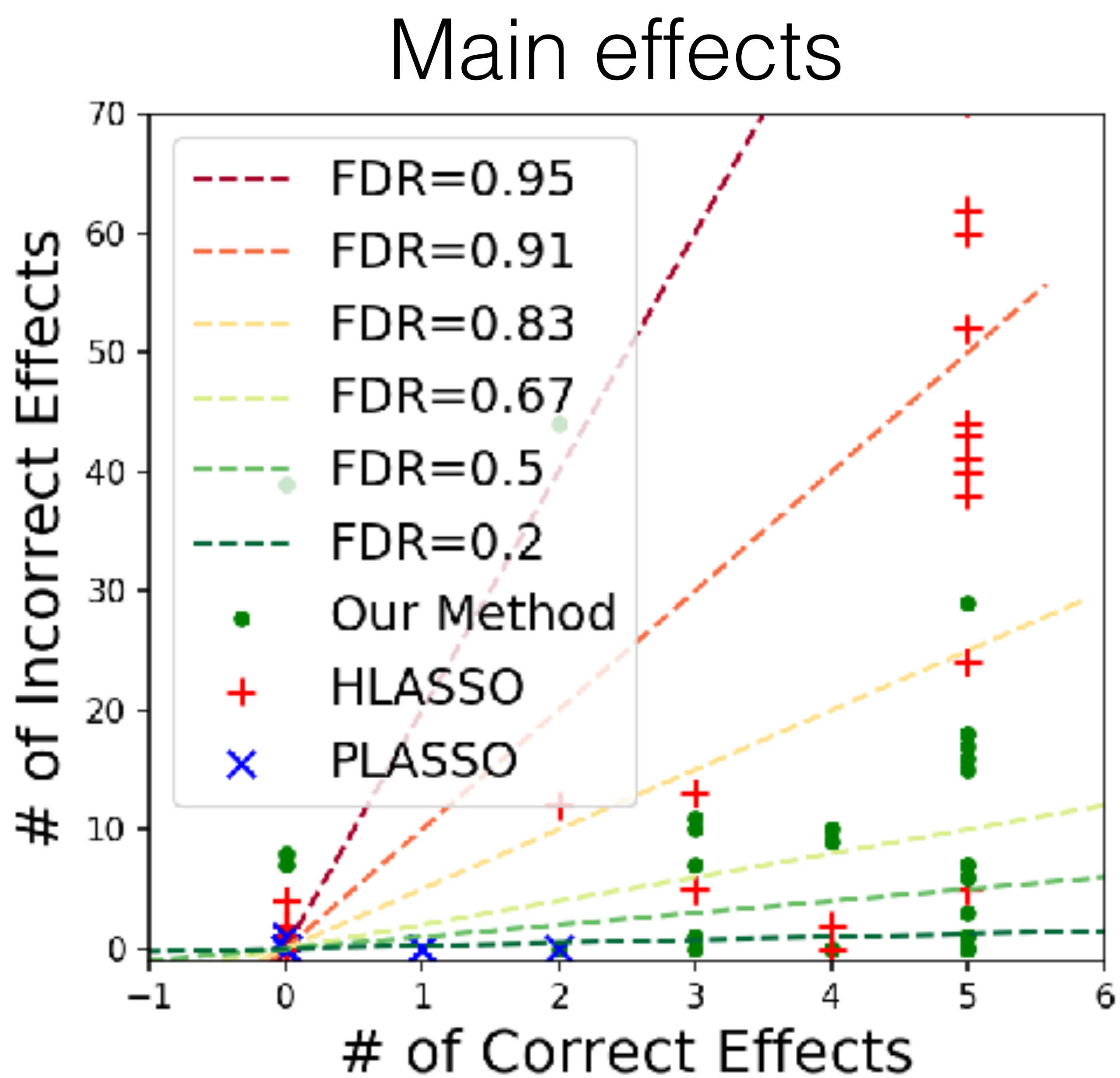

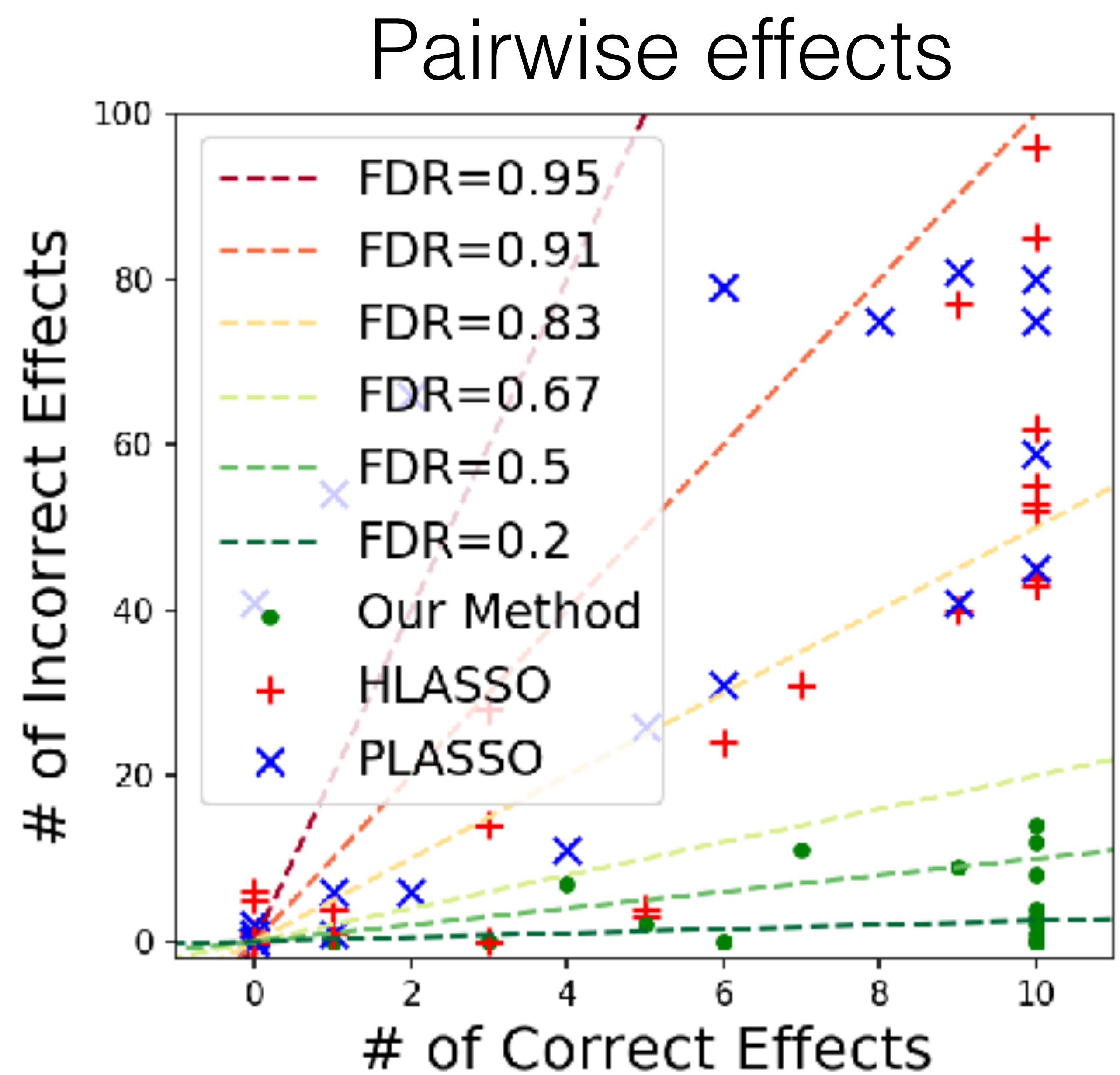

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METHOD	#MAIN	#PAIR
PLASSO	2 : 5	3 : 21

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METHOD	#MAIN	#PAIR
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HLASSO	**3 : 19**	**3 : 18**

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METHOD	#MAIN	#PAIR
PLASSO	4 : 0	2 : 78

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- Augment p with 200 fake (noise) covariates
  - 21,321 total parameters
- Key: (# original effects): (# of fake effects)
  - **No order** to blue: **lower** red is better

Method	#Main	#Pair
PLASSO	**4 : 0**	**2 : 78**
HLASSO	**6 : 46**	**4 : 38**

Experiments: Real data

- Covariates and response: Auto MPG
- N = 398, p = 6 (real-valued), but…
- Augment p with 200 fake (noise) covariates
  - 21,321 total parameters
- Key: (# original effects): (# of fake effects)
  - **No order** to blue: **lower** red is better

Method	#Main	#Pair
Our method	**3 : 0**	**1 : 0**
PLASSO	**4 : 0**	**2 : 78**
HLASSO	**6 : 46**	**4 : 38**

Conclusions

We provide: fast, accurate detection of pairwise interactions

R Agrawal, BL Trippe, JH Huggins, and T Broderick. The Kernel interaction trick: Fast Bayesian discovery of pairwise interactions in high dimensions. *ICML* 2019. ArXiv:1905.06501

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- In Pyro: `http://pyro.ai/numpyro/sparse_regression.html`

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We provide: fast, accurate detection of pairwise (and higher-order) interactions

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- Response types (binary, count, etc) & nonlinearity

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JH Huggins, T Campbell, M Kasprzak, and T Broderick. Scalable Gaussian process inference with finite-data mean and variance guarantees. *AISTATS* 2019.

R Agrawal, T Campbell, JH Huggins, and T Broderick. Data-dependent compression of random features for large-scale kernel approximation. *AISTATS* 2019.

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Up next:

- Response types (binary, count, etc) & nonlinearity
- Improve scaling in N
- Applications!

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More in the Broderick Group

L Masoero, F Camerlenghi, S Favaro, T Broderick. More for less: Predicting and maximizing variant discovery under a fixed budget via Bayesian nonparametrics. https://arxiv.org/abs/1912.05516

- For fixed budget, there is trade-off in sequencing more genomes and sequencing at greater depth
- We provide new method for prediction of # new variants and optimal allocation of more genomes vs. depth
  - Lowest error when using pilot TCGA dataset to predict the number of new variants to be observed in the follow-up MSK-impact dataset (N=9593) across 197 highly variable, cancerous genes
  - (Only) our prediction can handle when sequencing depth changes between pilot and follow-up study
  - (Only) our method optimizes under fixed budget

T Broderick, R Giordano, R Meager. An Automatic Finite-Sample Robustness Metric: Can Dropping a Little Data Change Conclusions? In preparation.