Fast Discovery of Pairwise Interactions in High Dimensions using Gaussian Processes

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Associate Professor
EECS, MIT

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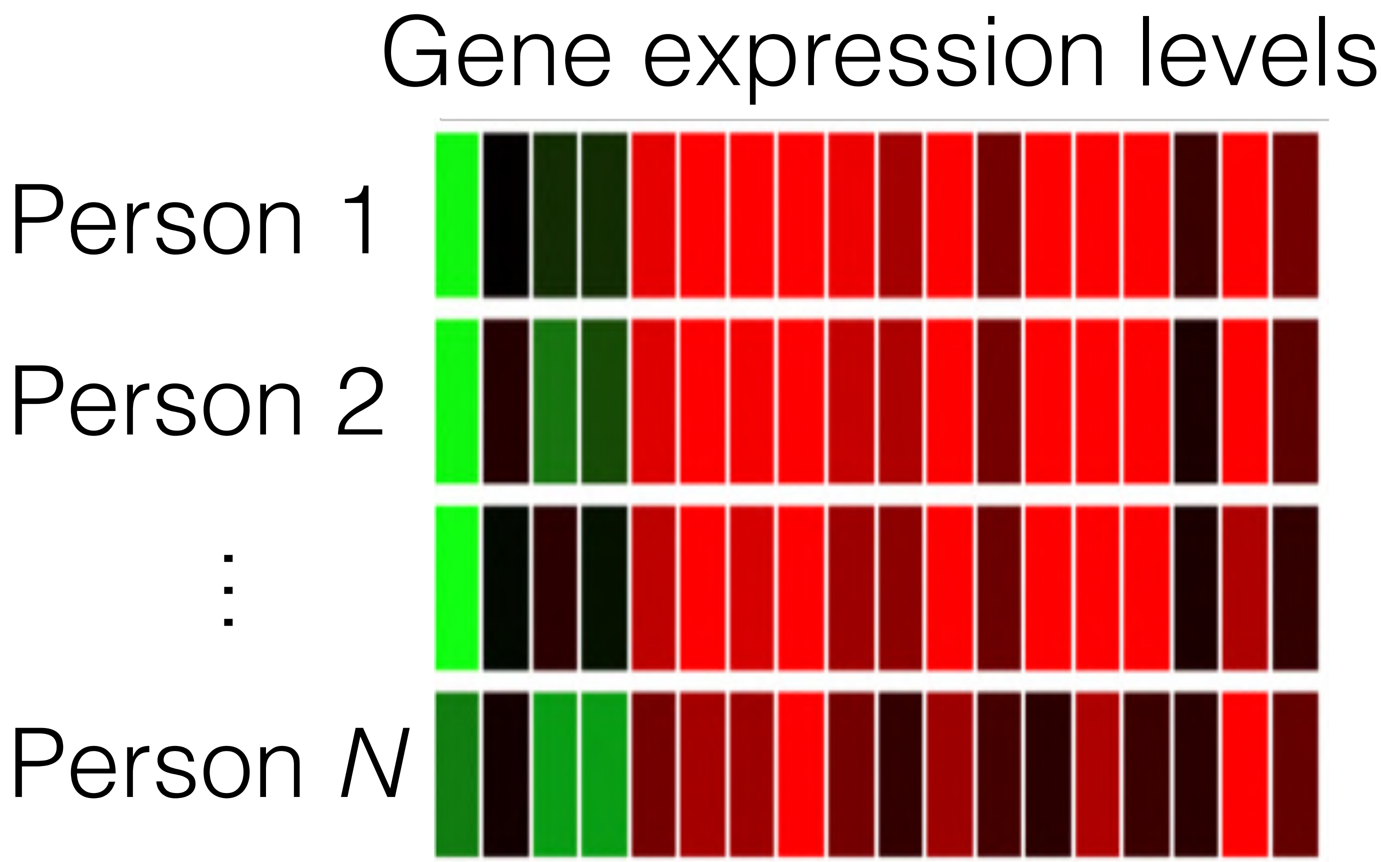
Gene expression levels
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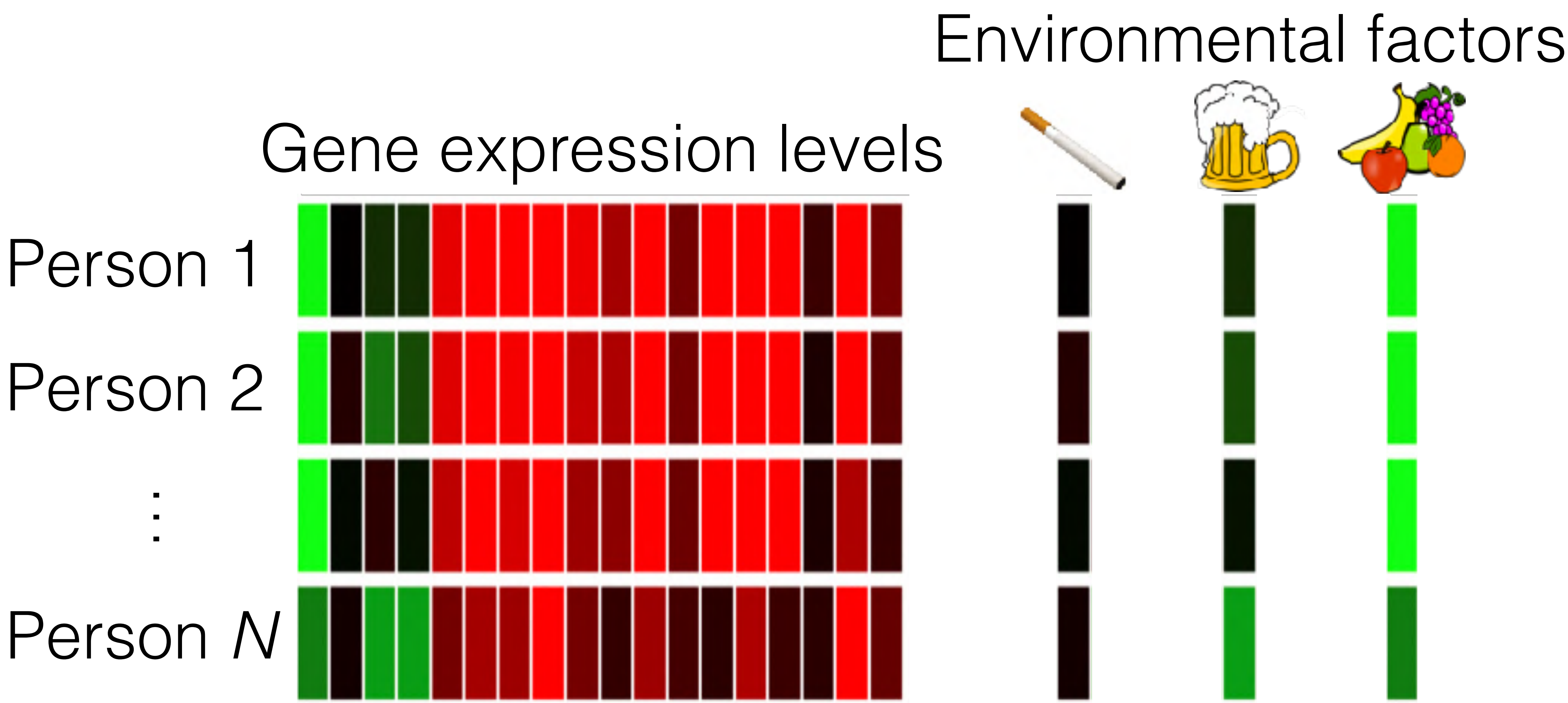
Person 2
⋮
Person N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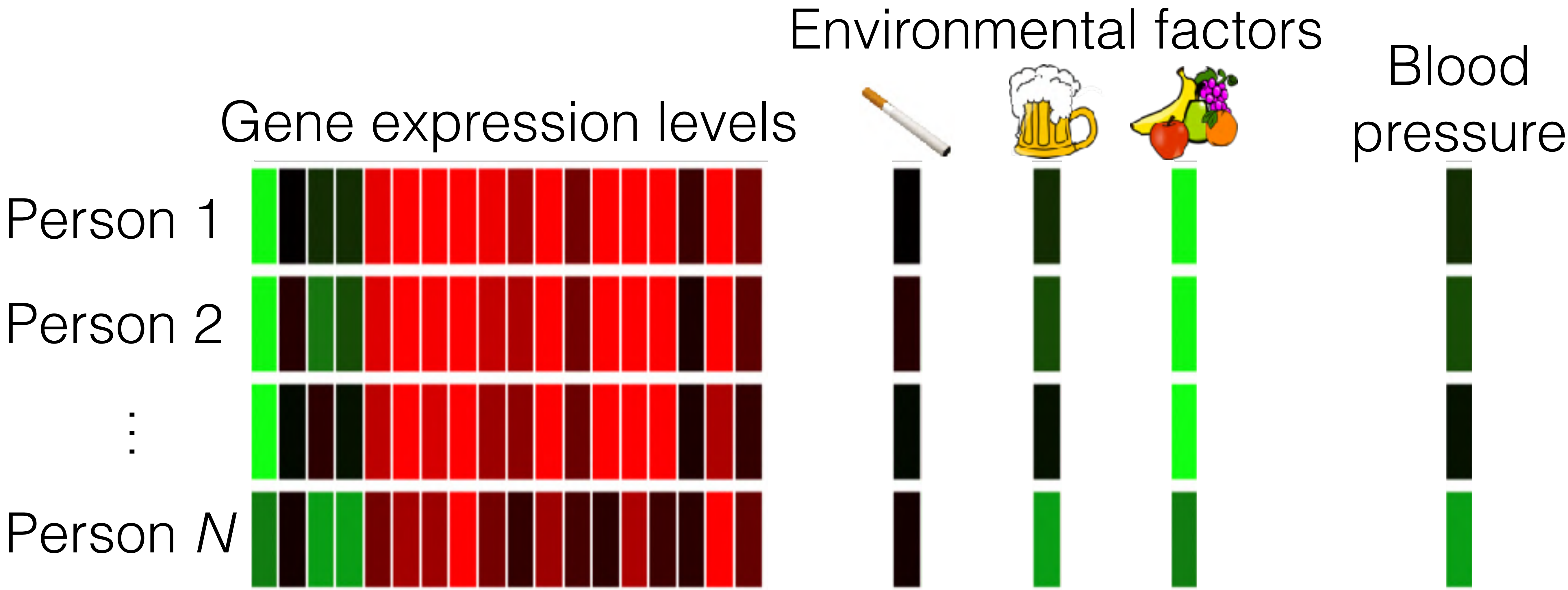
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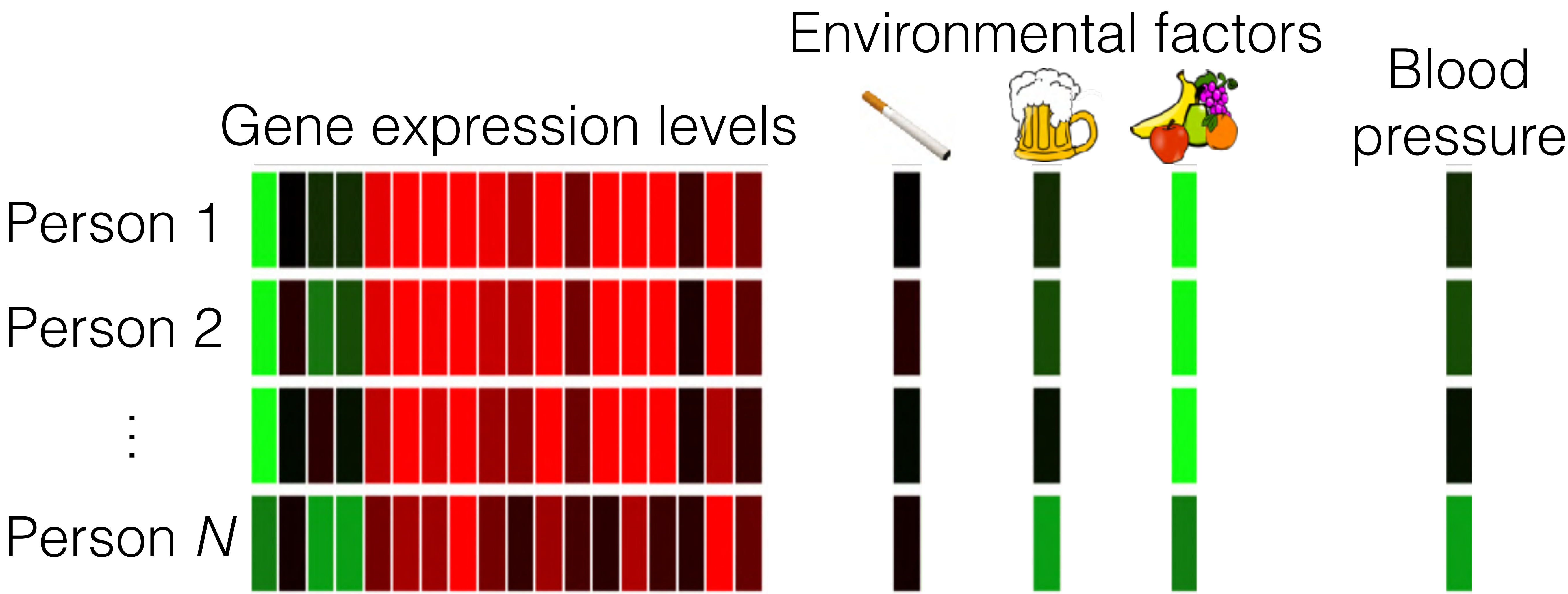

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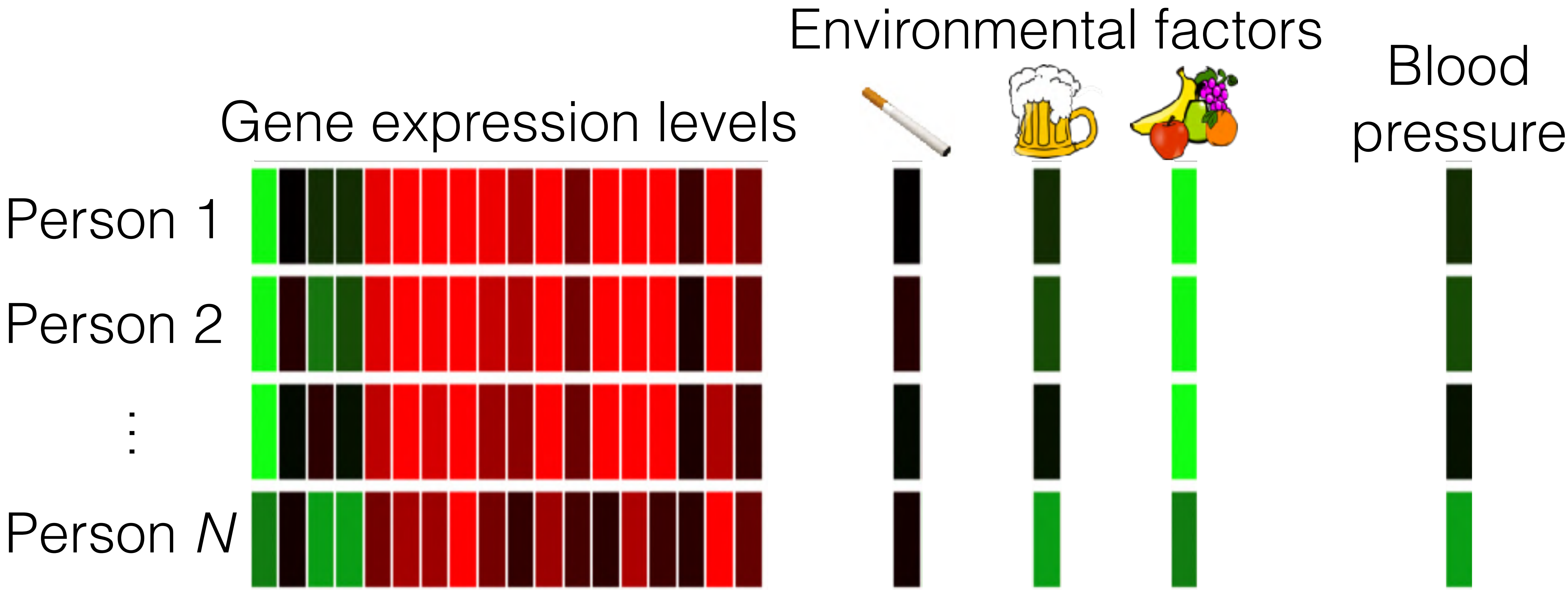

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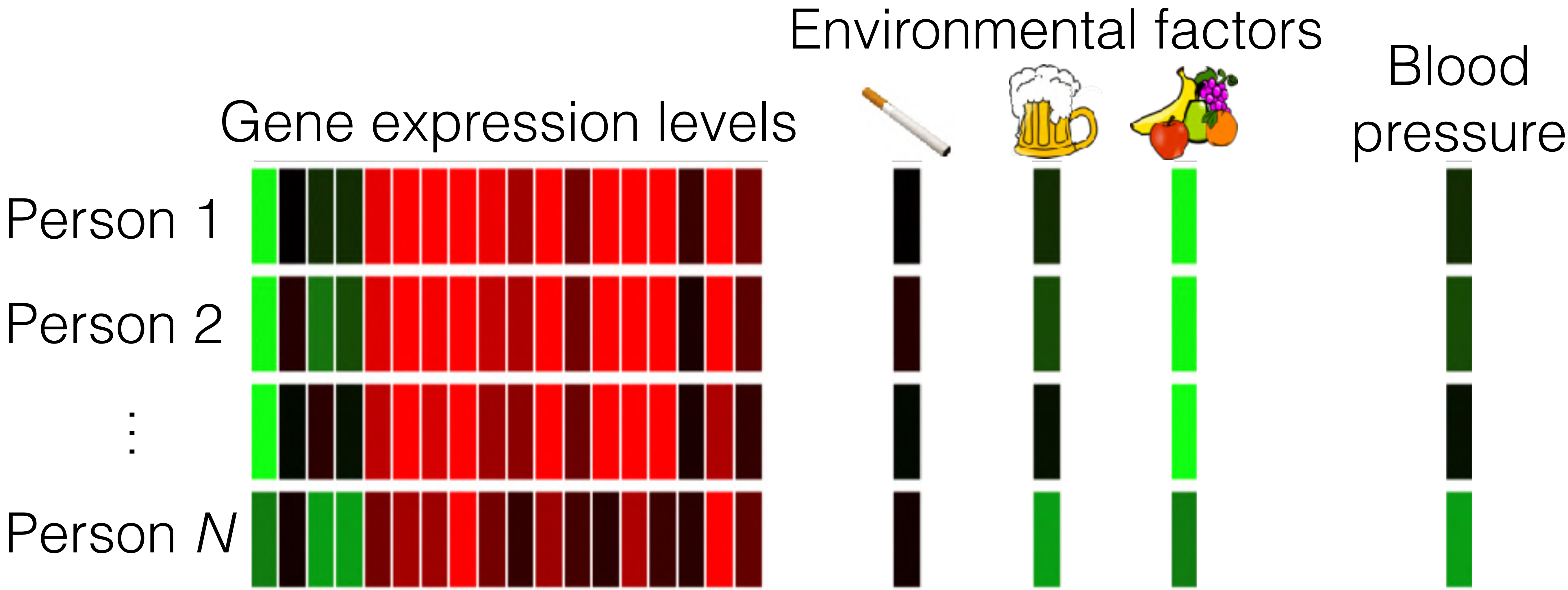

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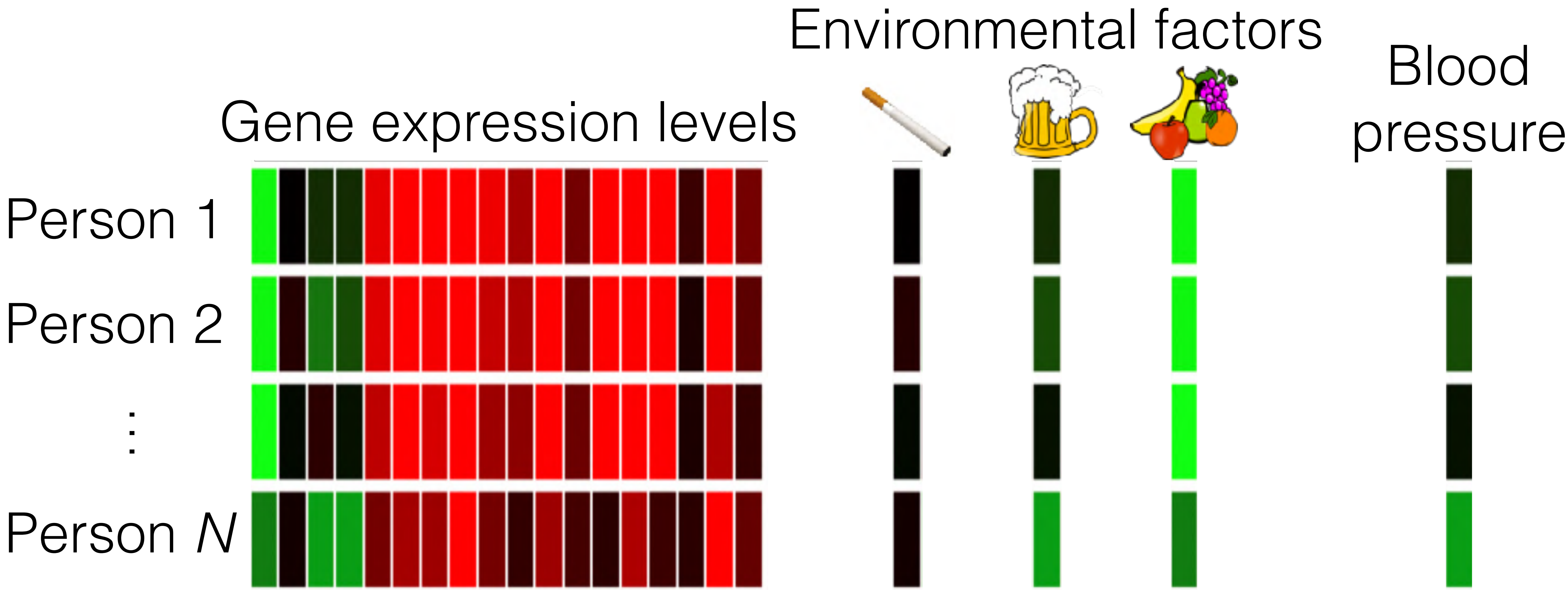

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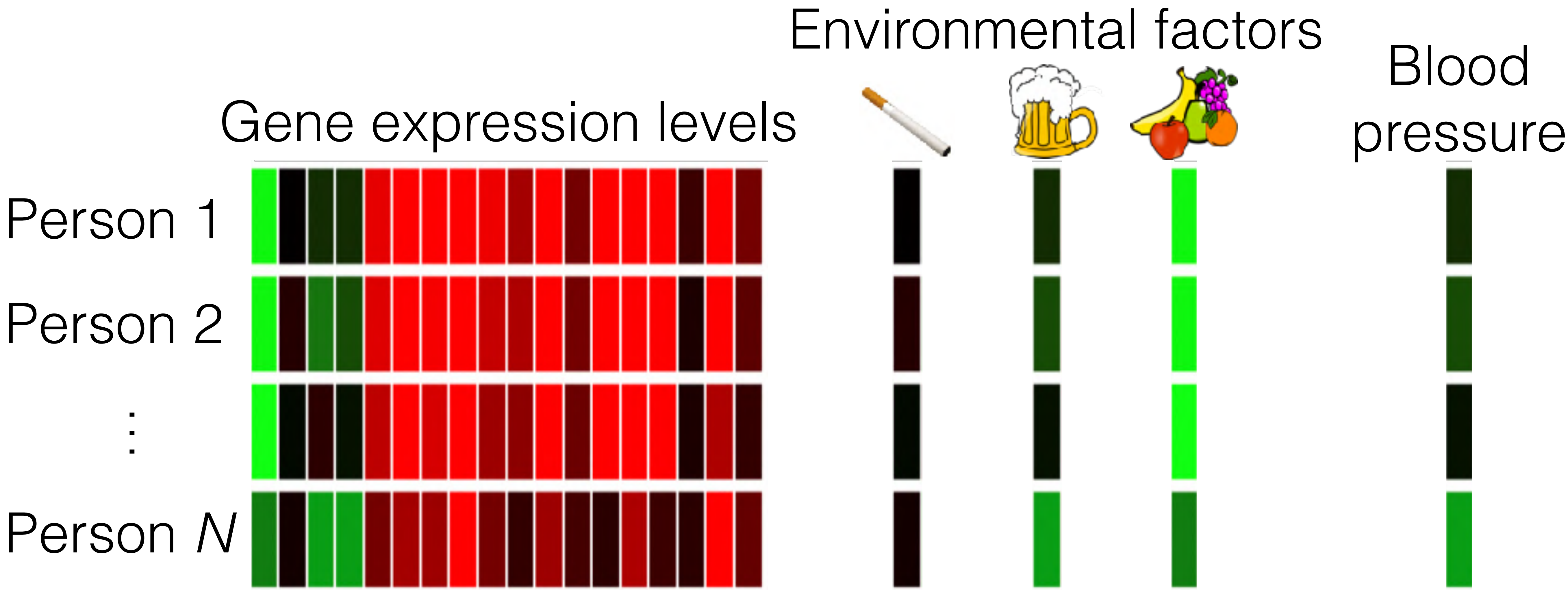

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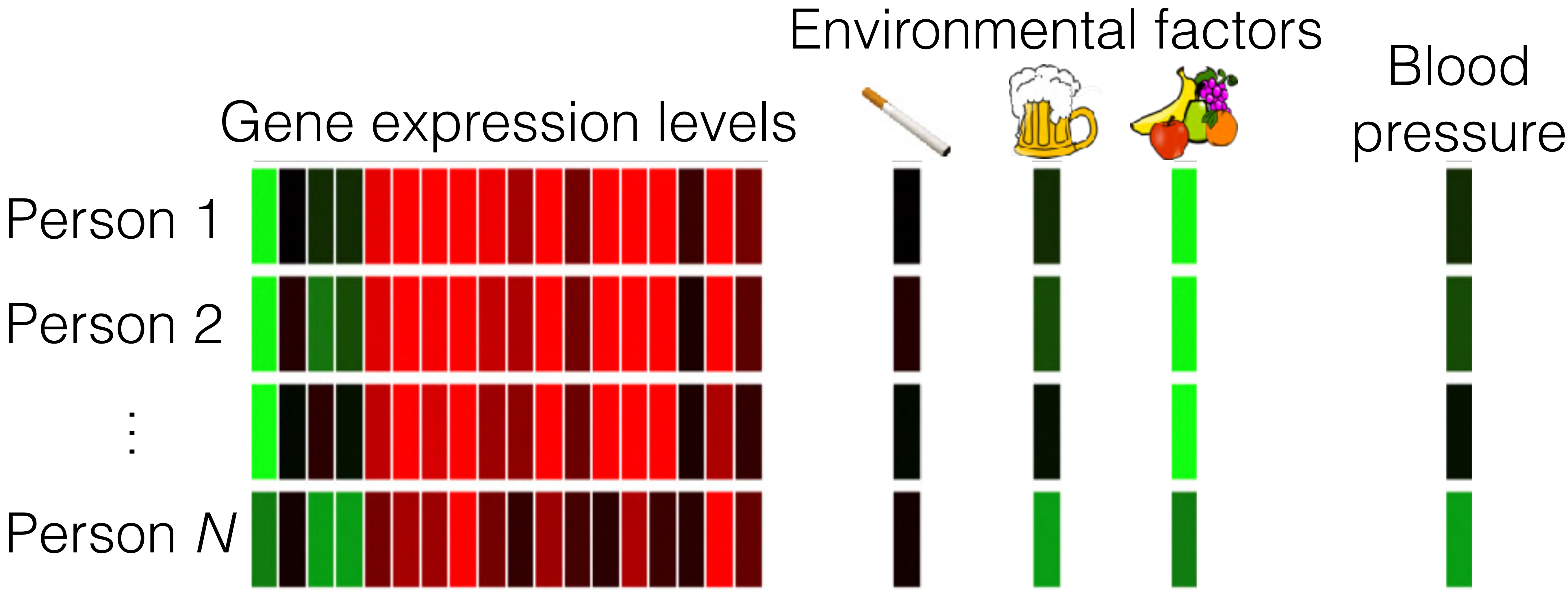

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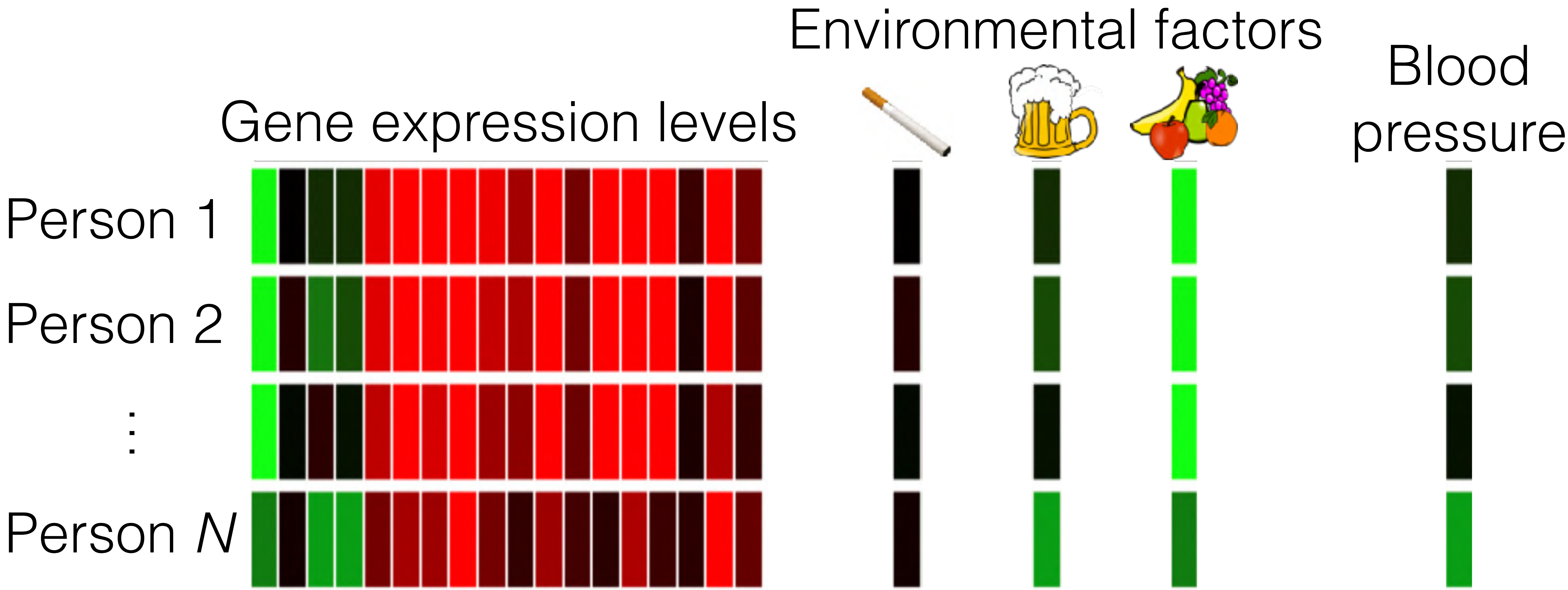

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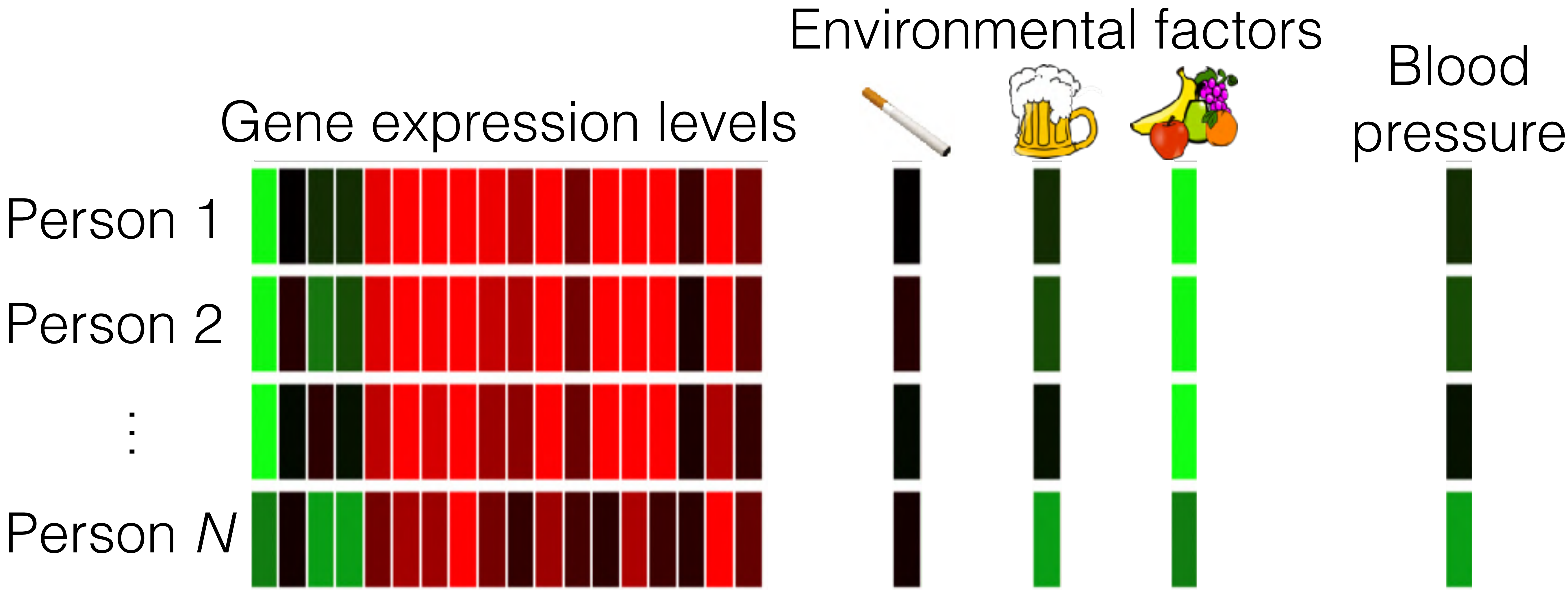

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  - Better scaling in p & better accuracy than LASSO-based methods. Orders of magnitude faster than naive Bayesian inference

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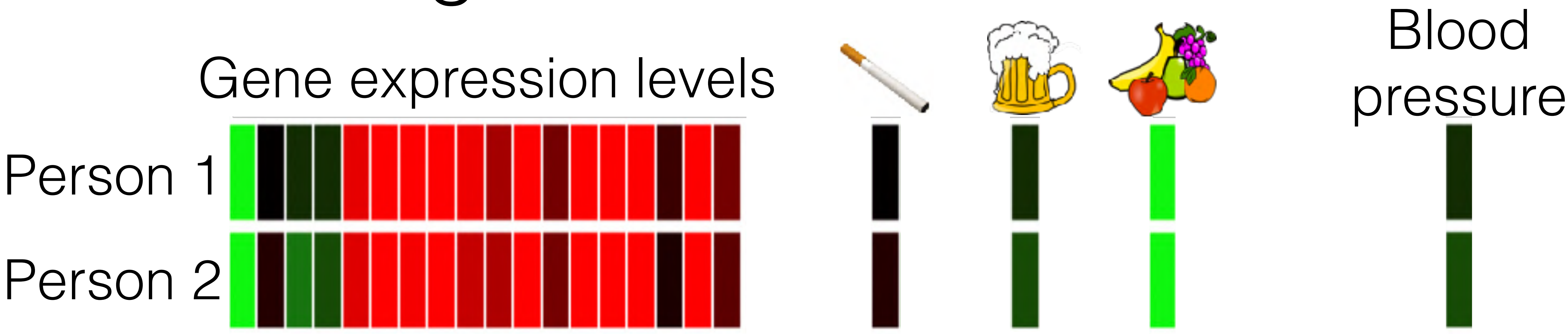

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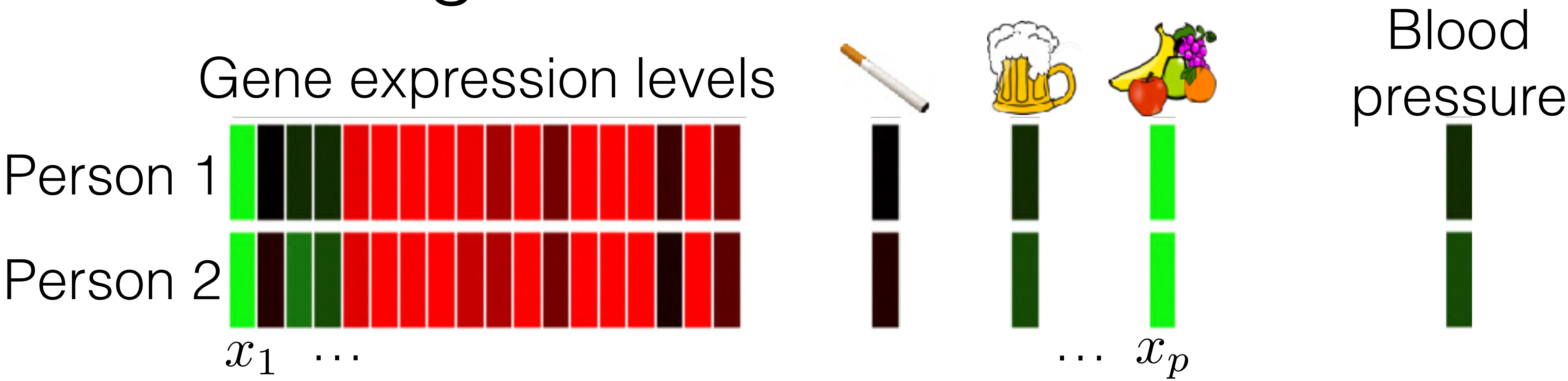

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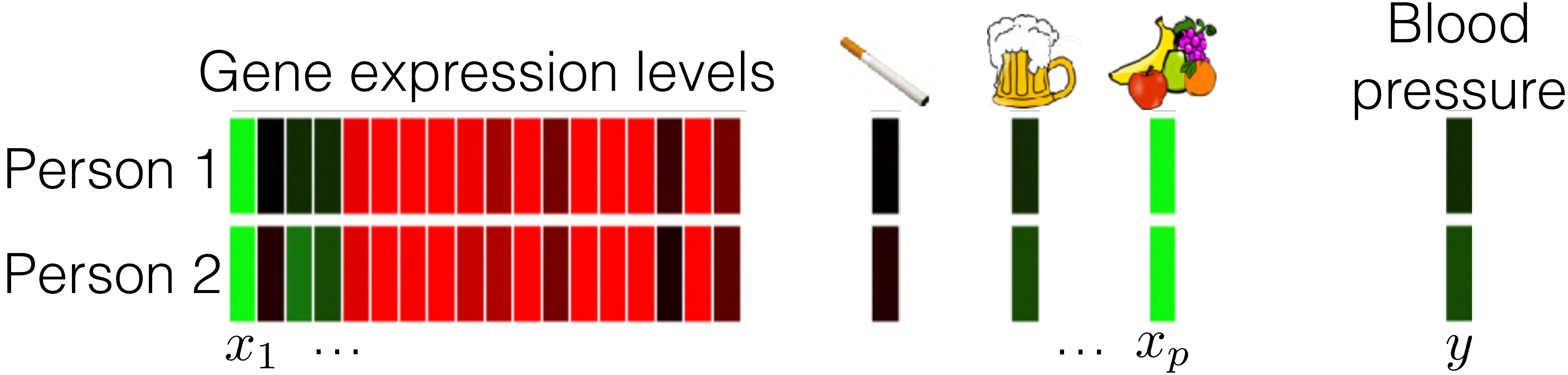

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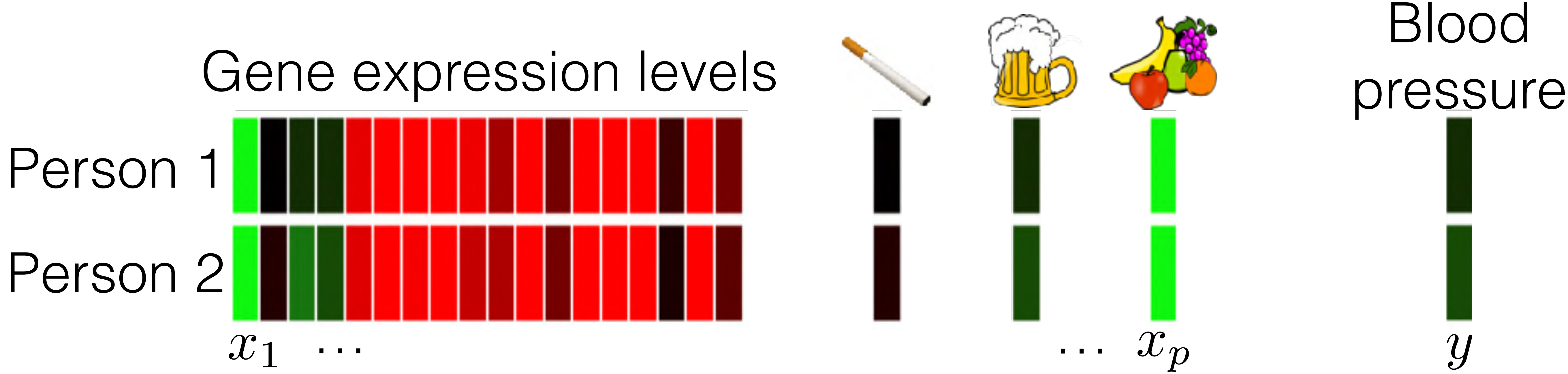

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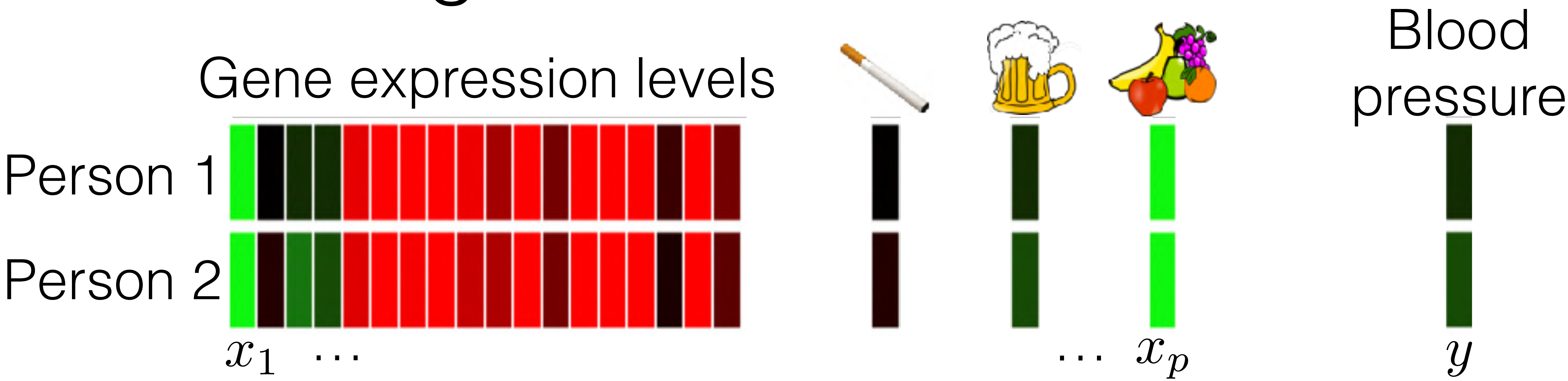

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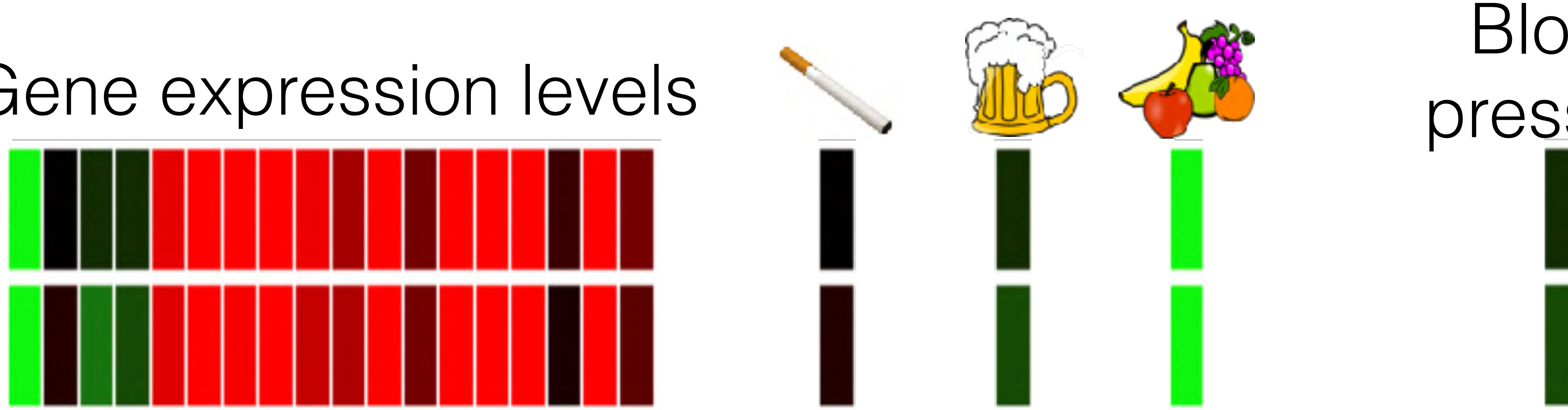

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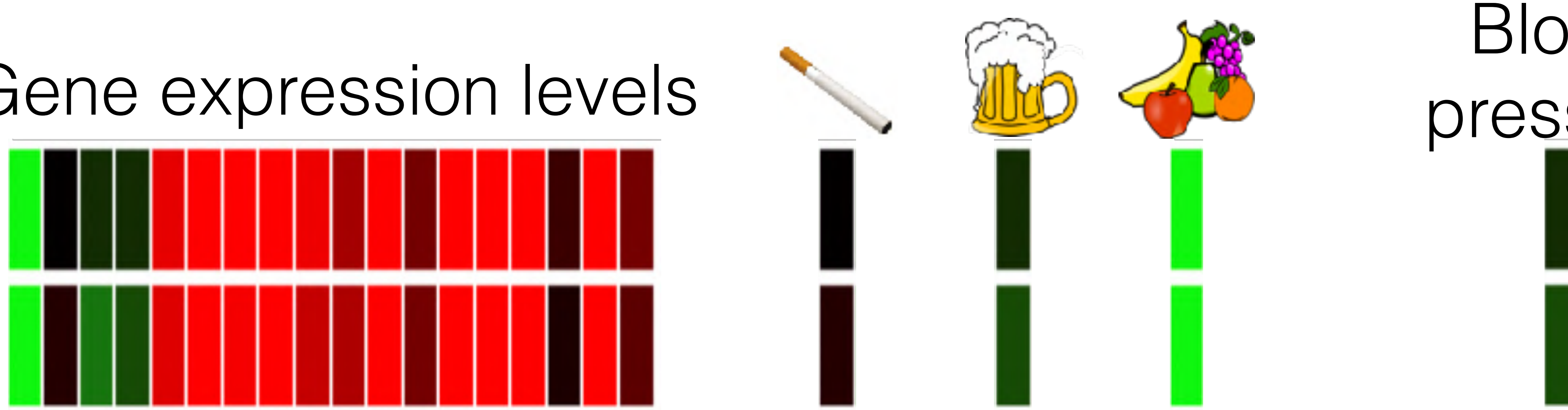

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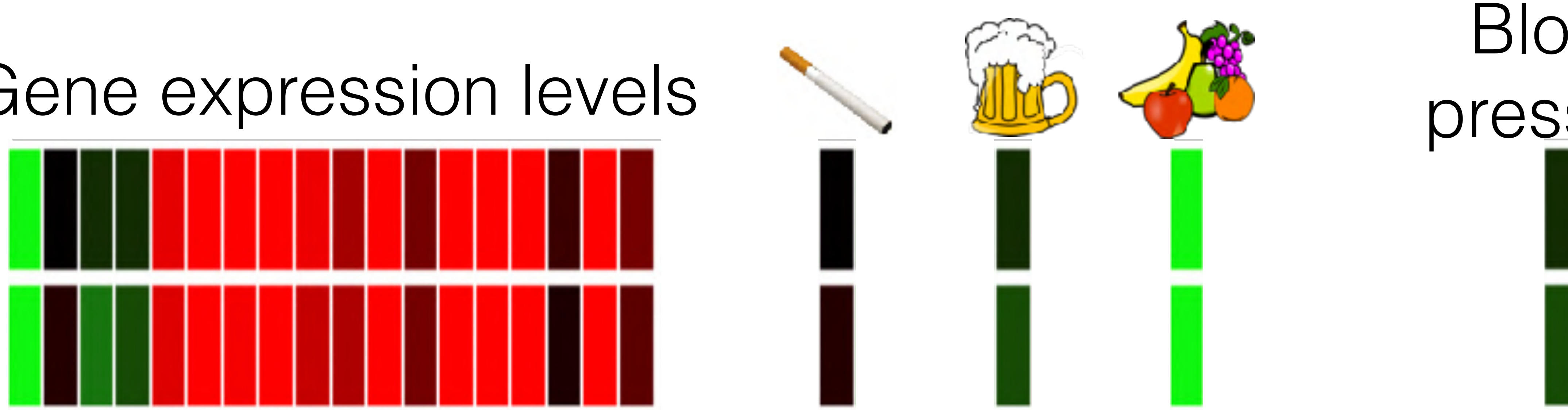

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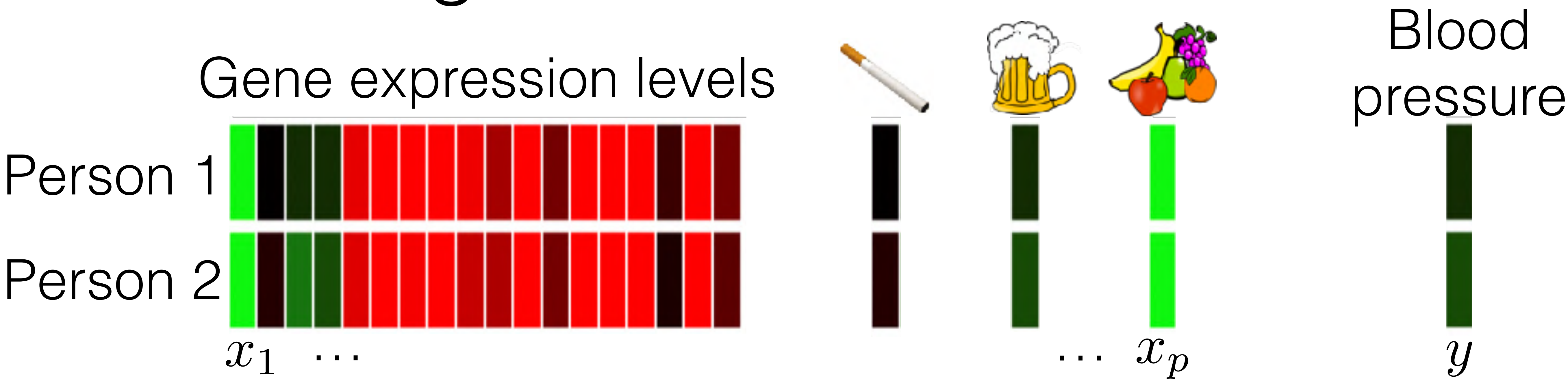

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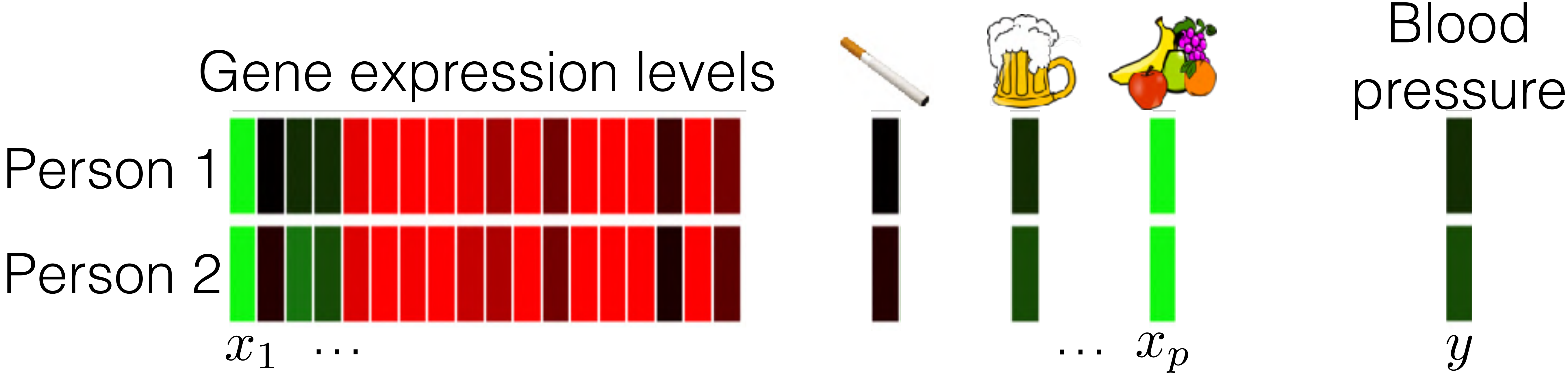

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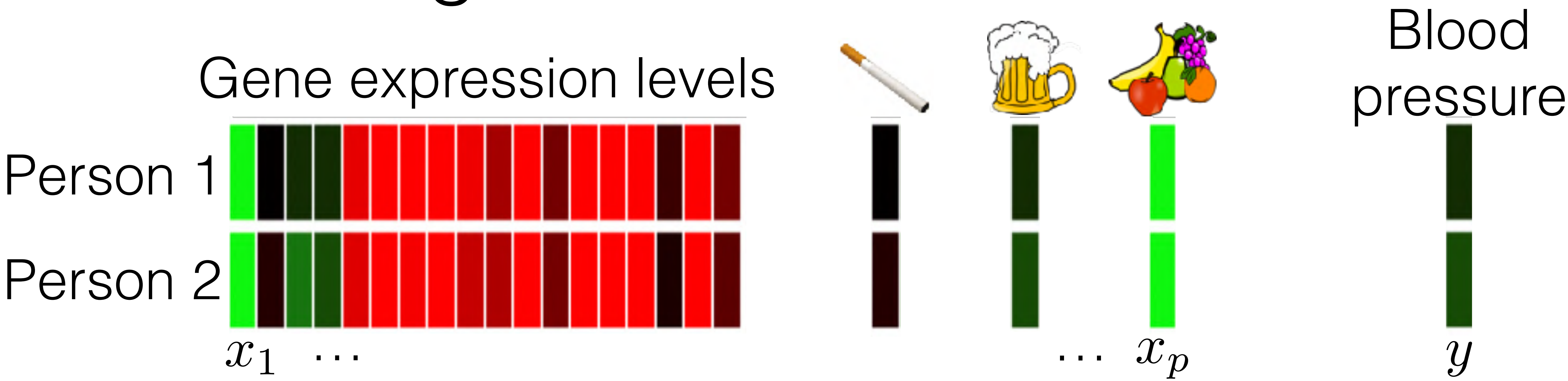

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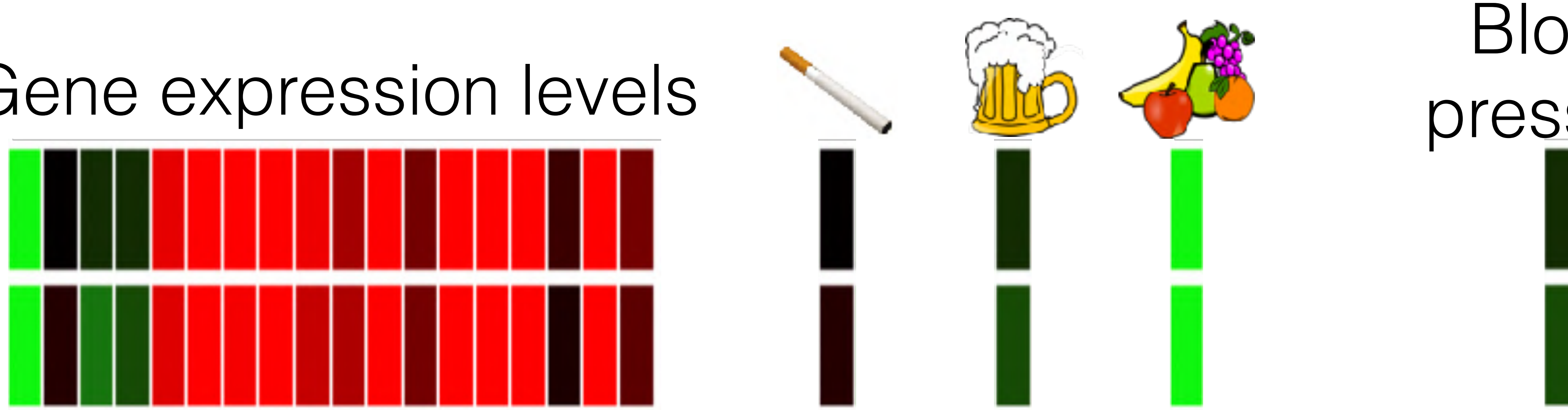

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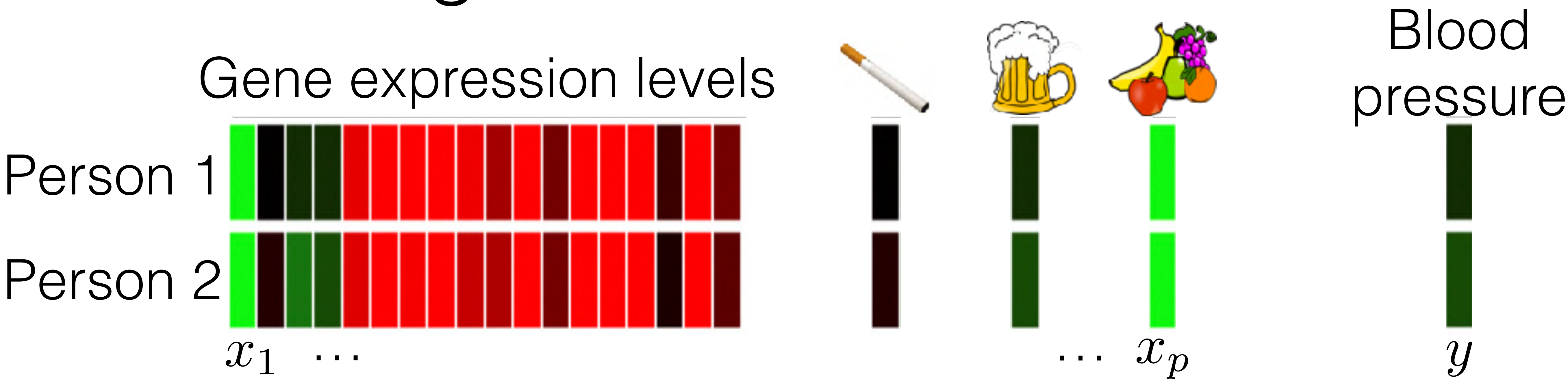

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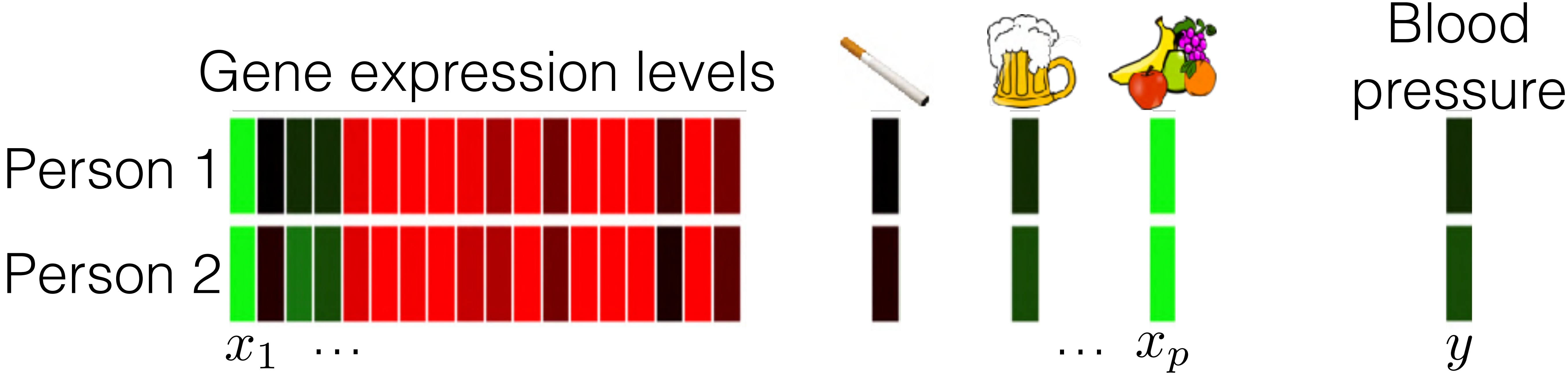

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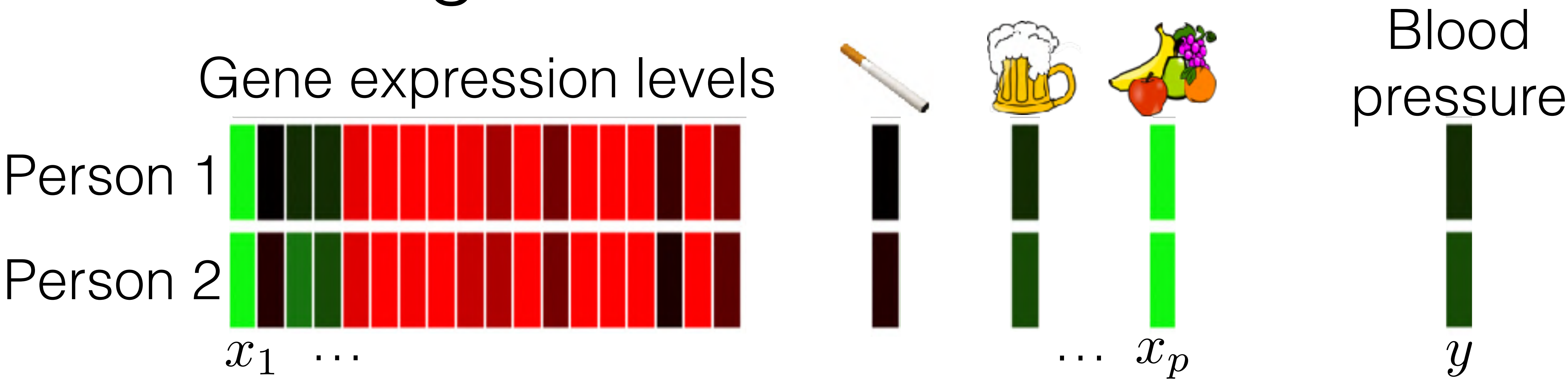

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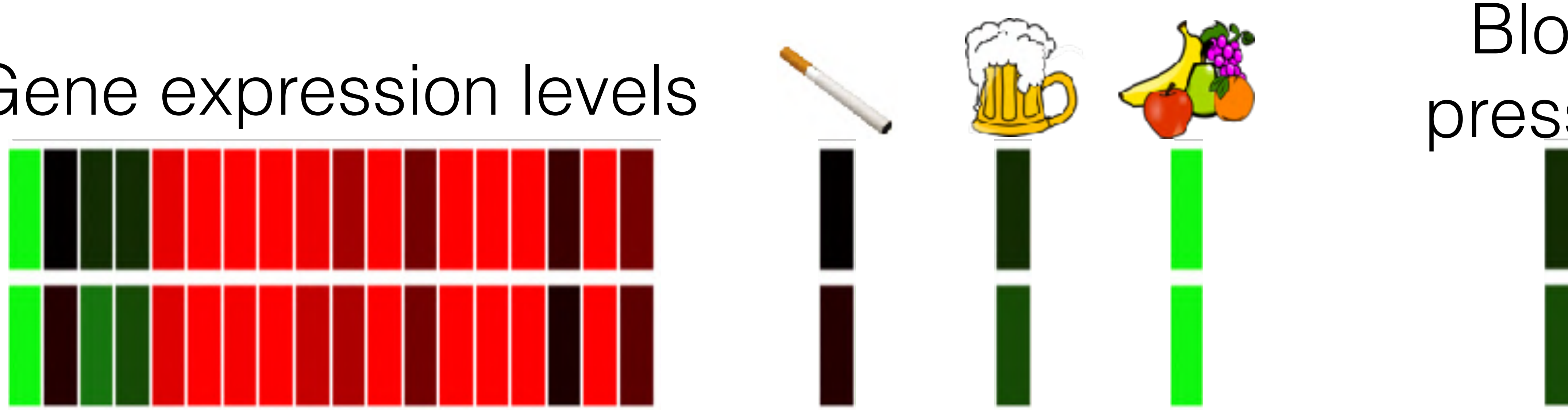

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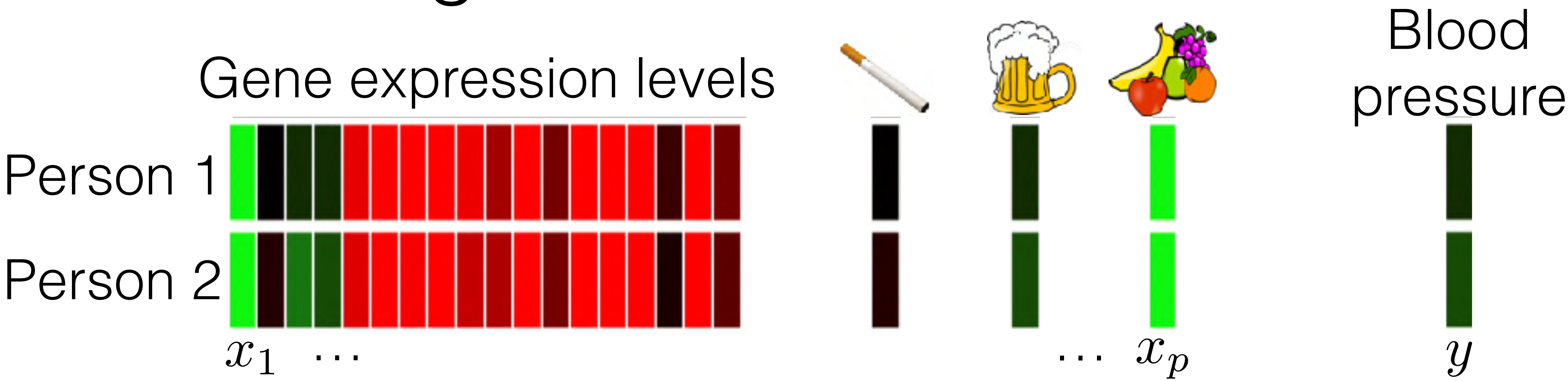

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- **Our solution**: using structure in covariates + sparsity assumptions to reduce to a problem *linear* in p

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Not just for SKIM

Kernel Interaction Sampler vs. Naive MCMC

- MCMC option 1: sample θ

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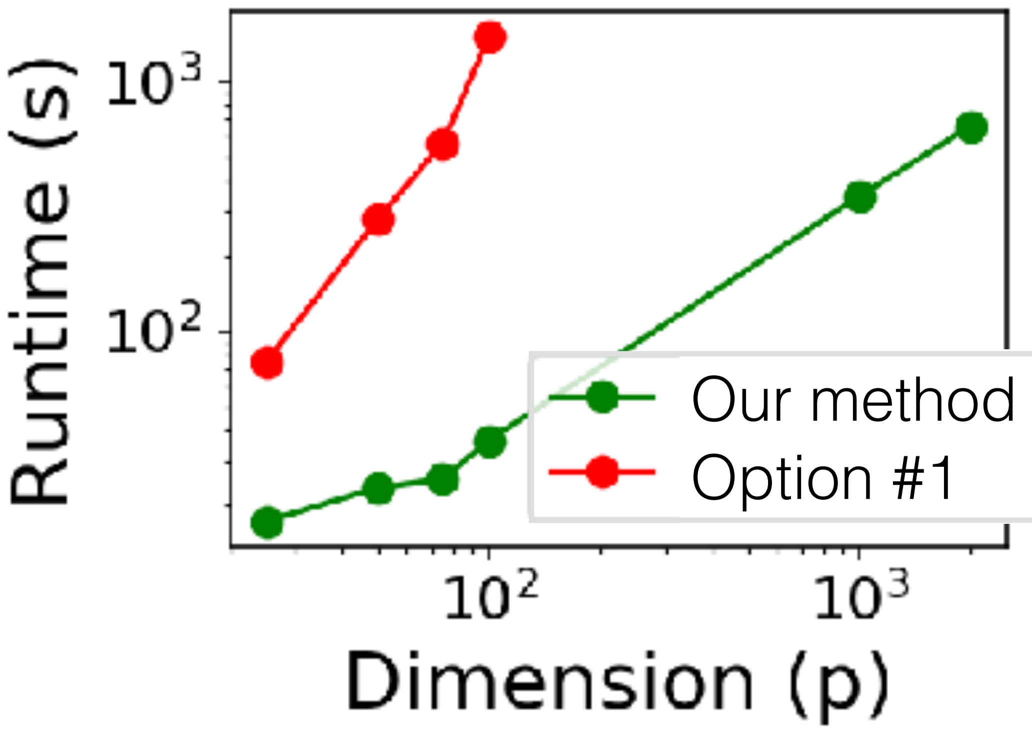

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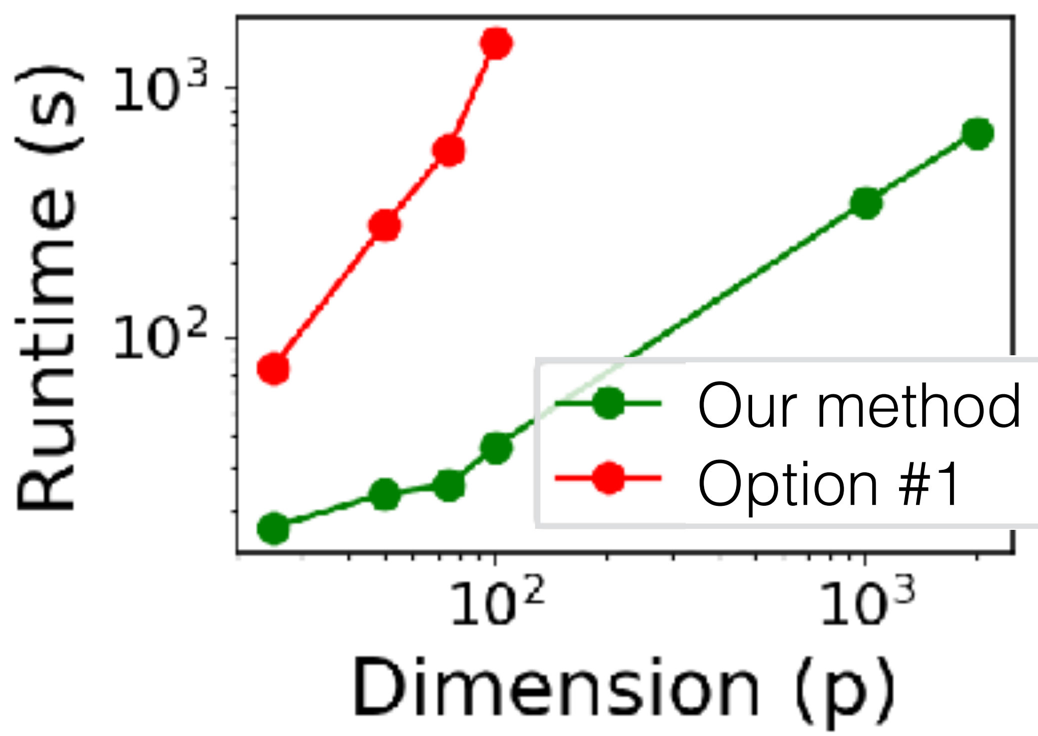

- Mixing (1000 iters Stan):
  - Option #1: all $\hat{R}$ > 1.05
  - Our method: all $\hat{R}$ < 1.05

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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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X: *N*×*p*

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$\boldsymbol{\Phi}_2$: $N \times p^2$

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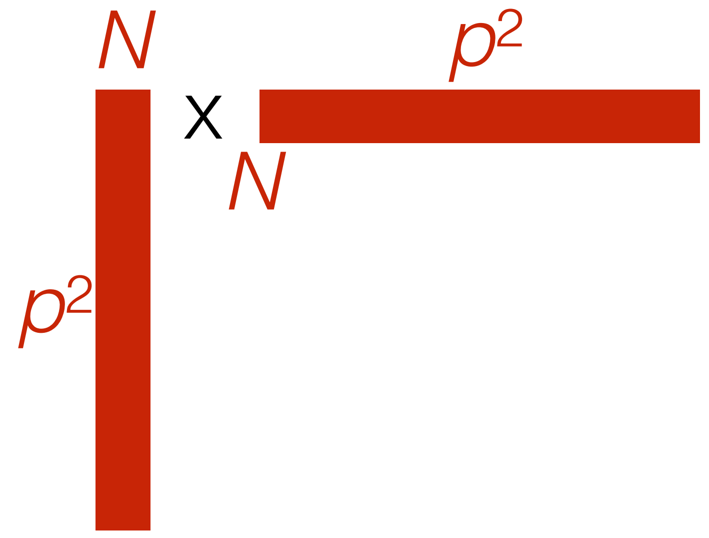

Kernel Interaction Sampler vs. Naive MCMC

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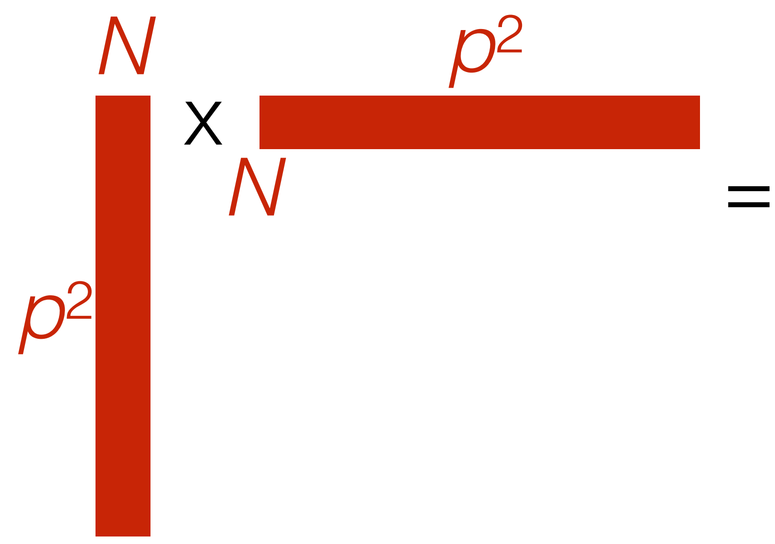

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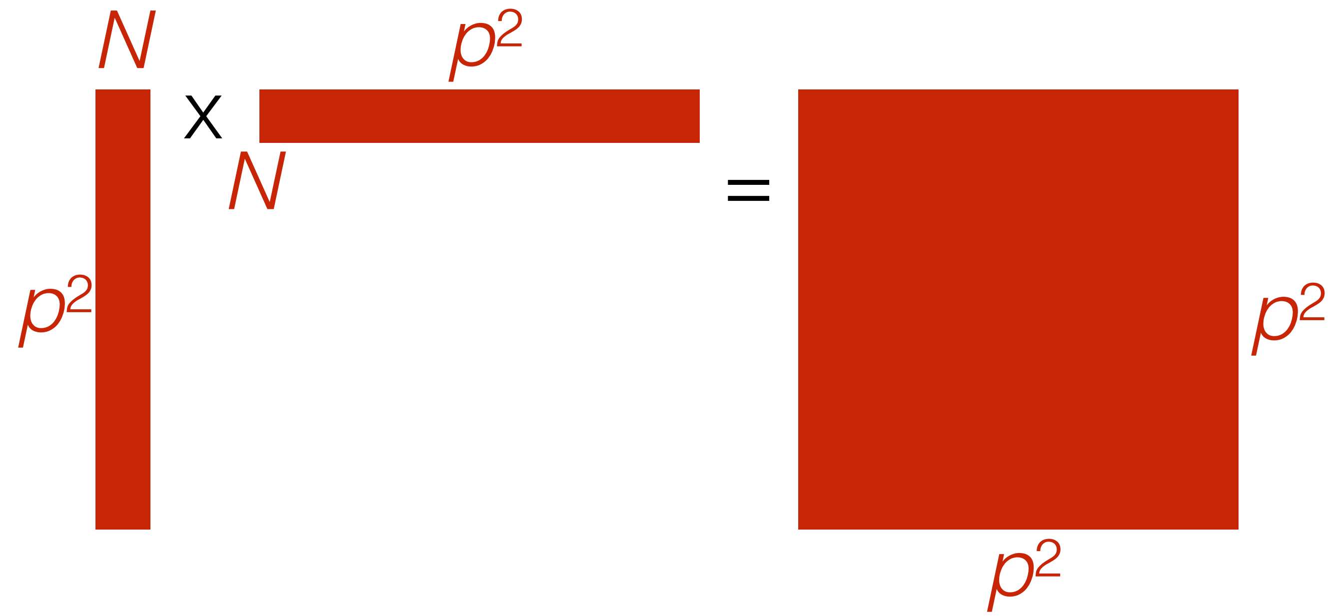

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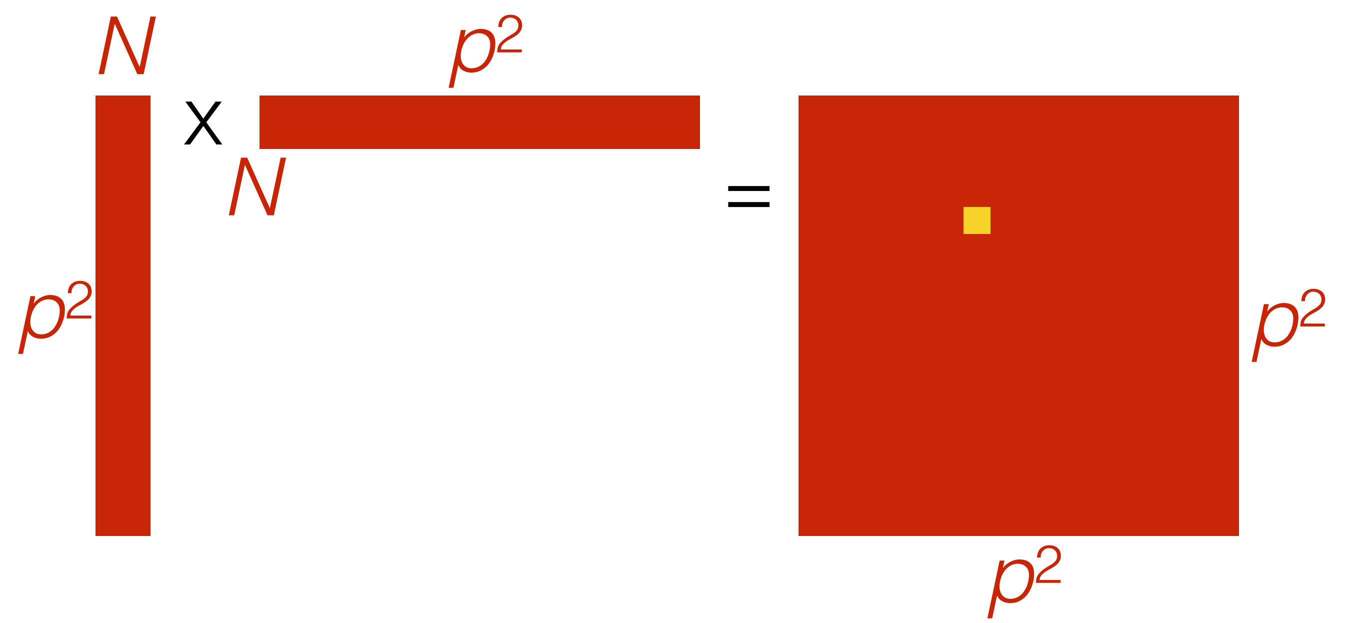

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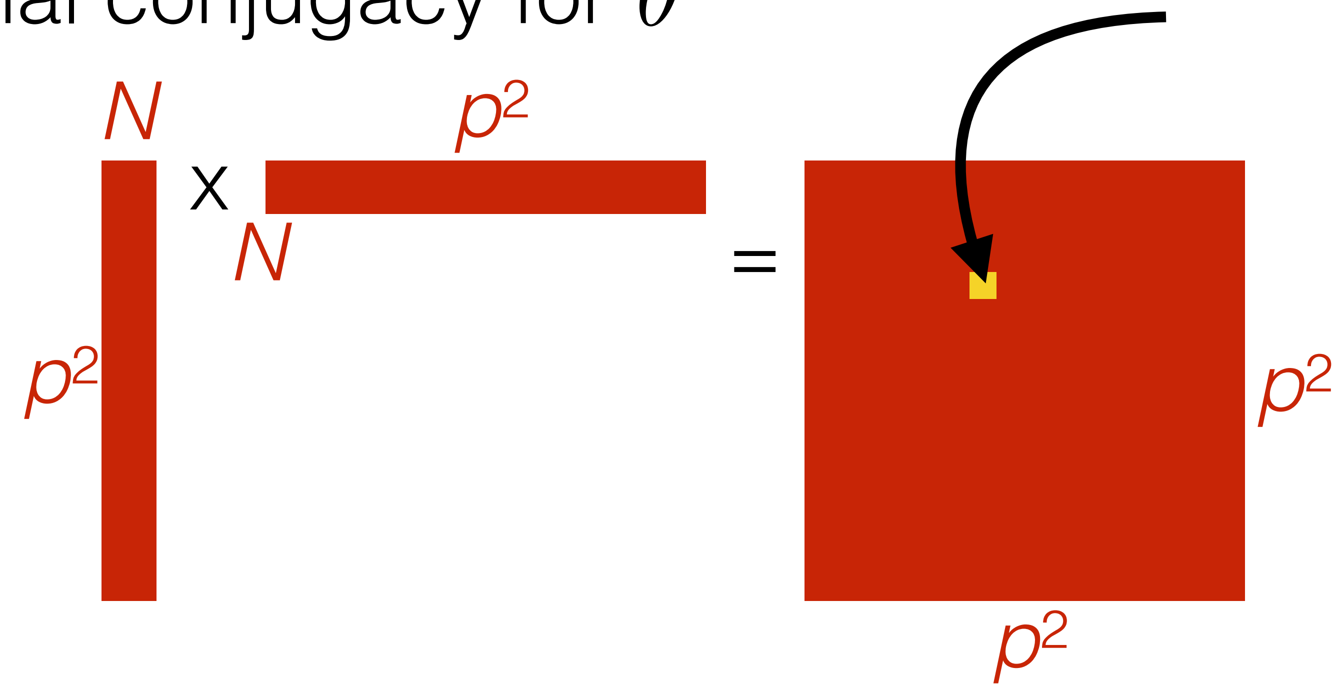

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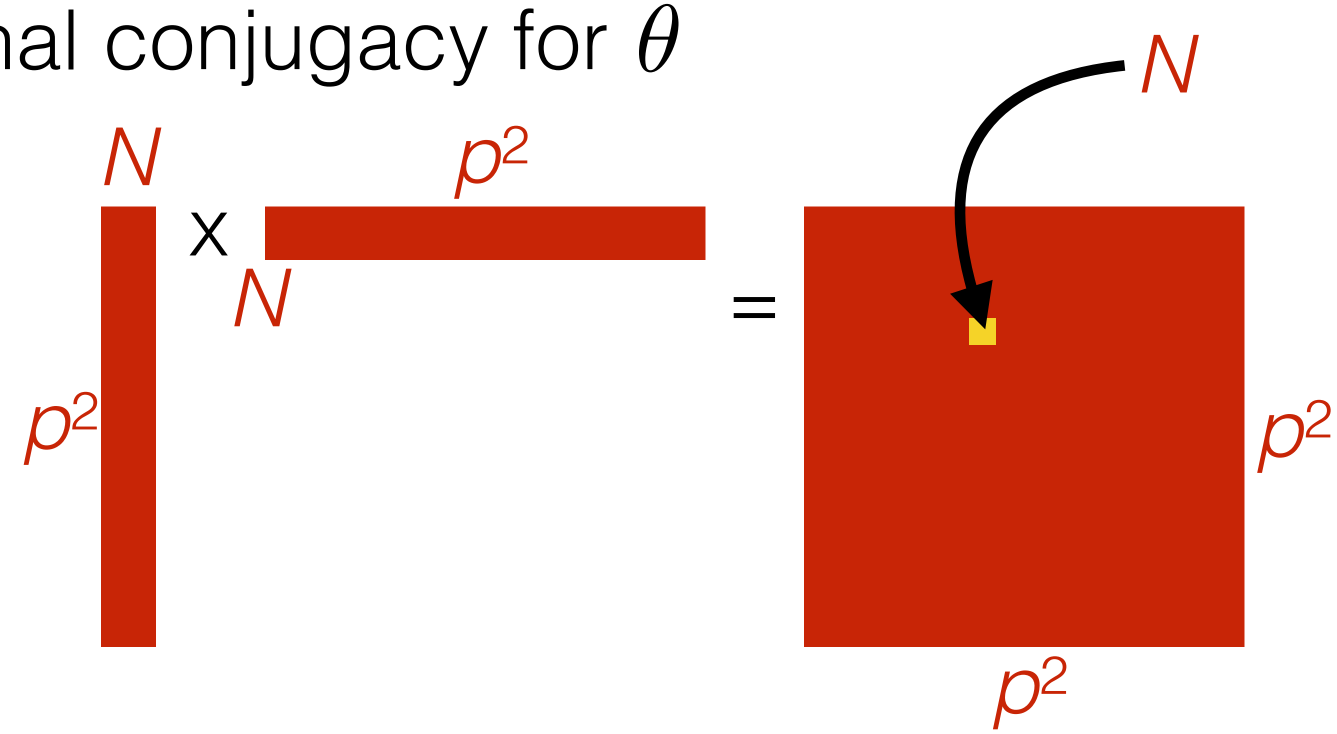

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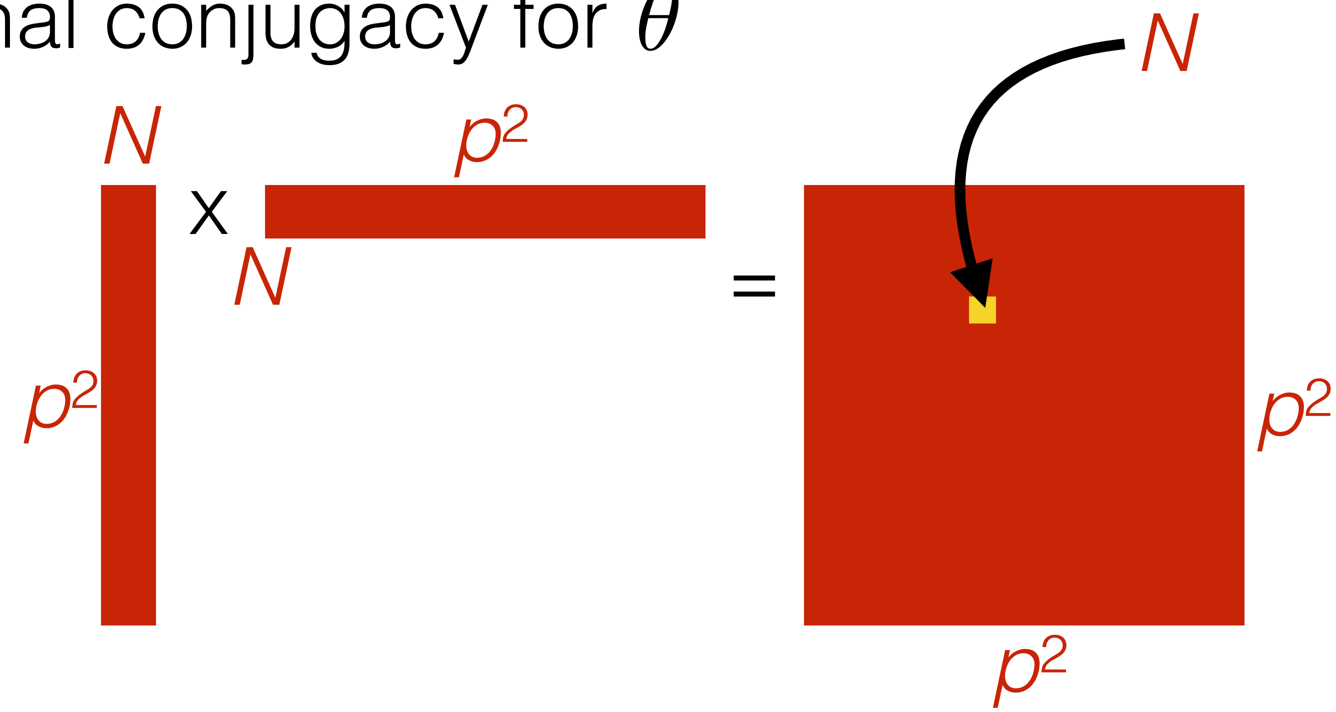

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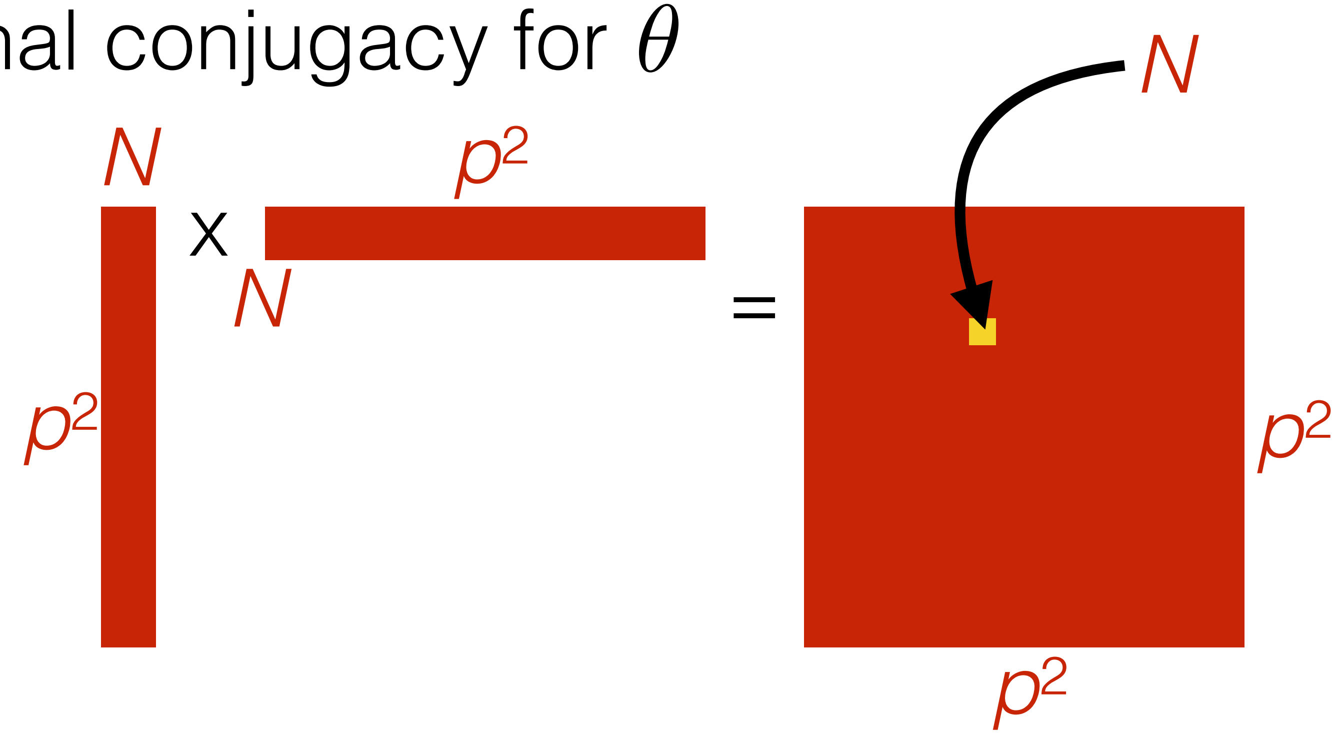

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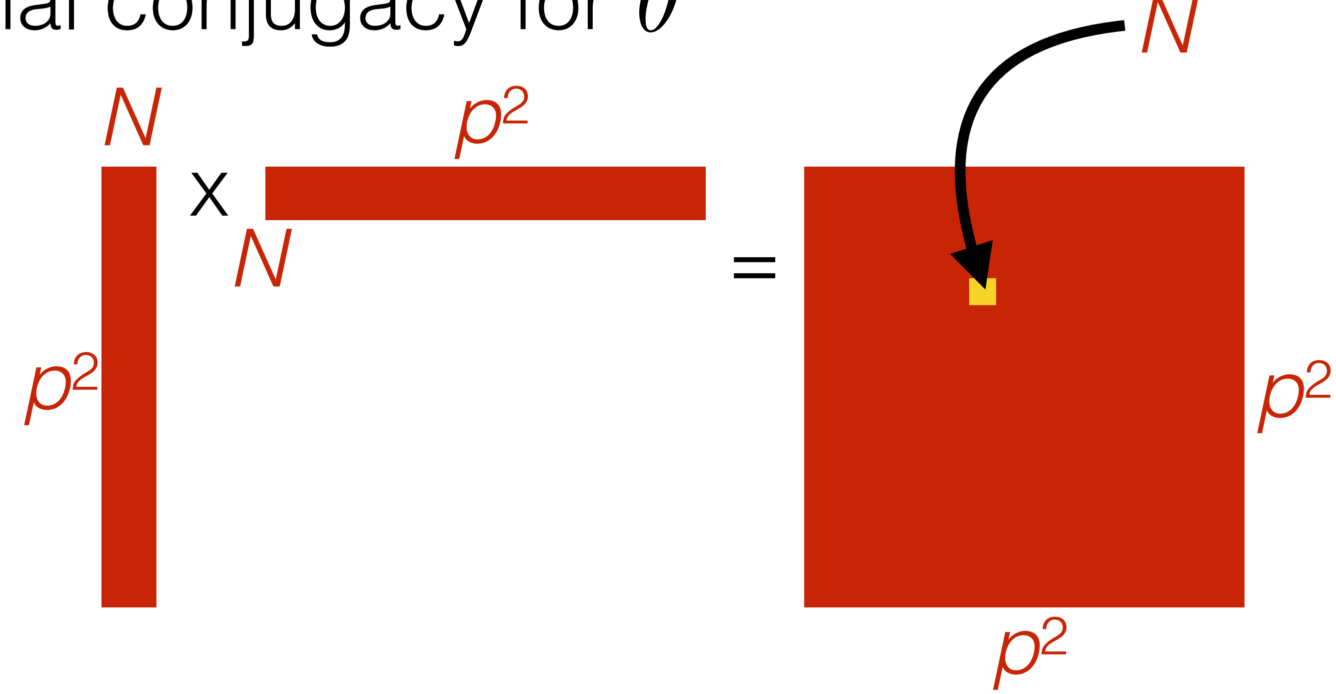

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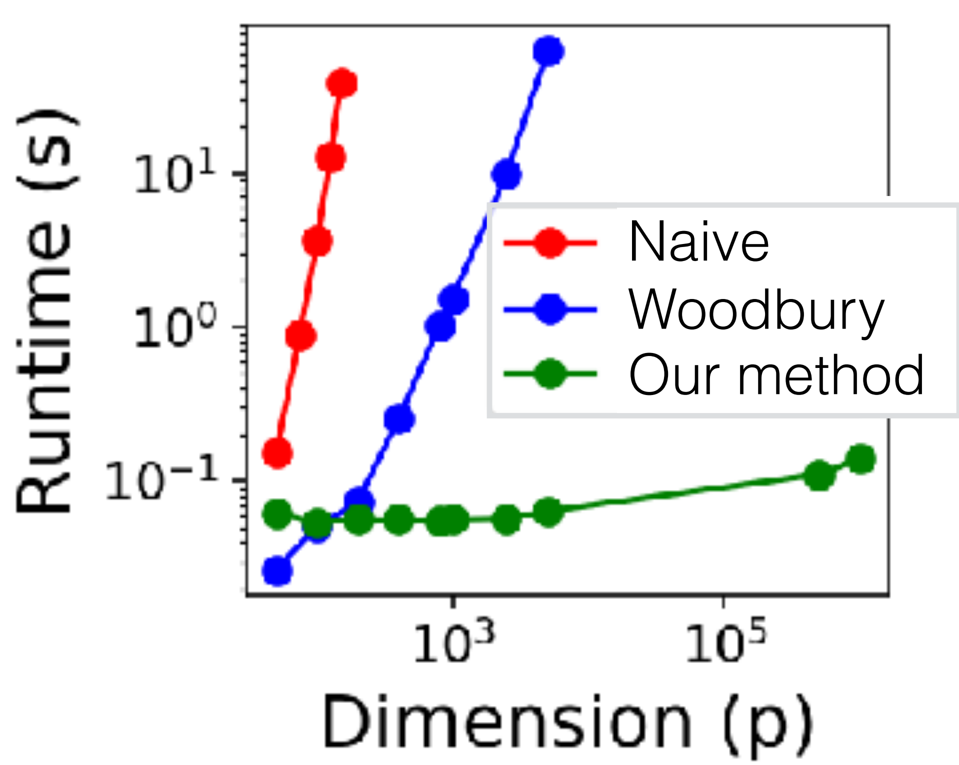

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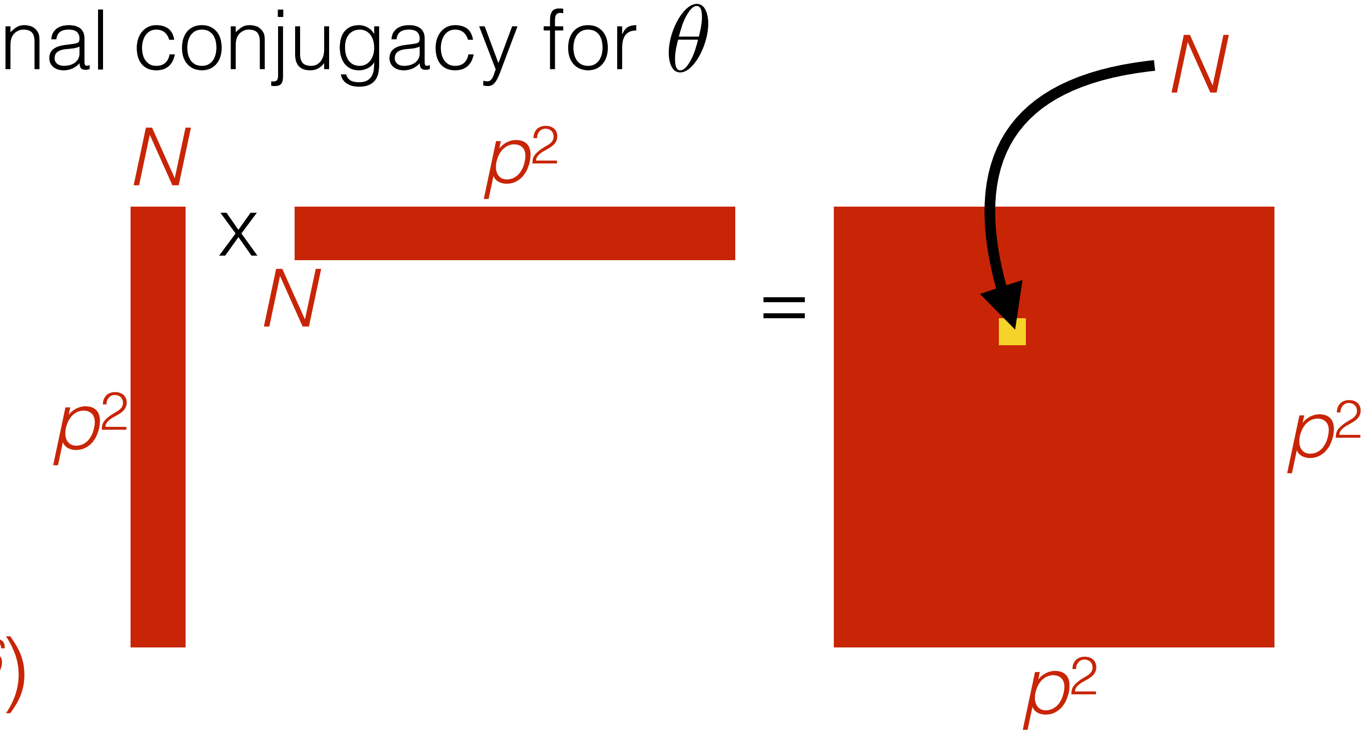

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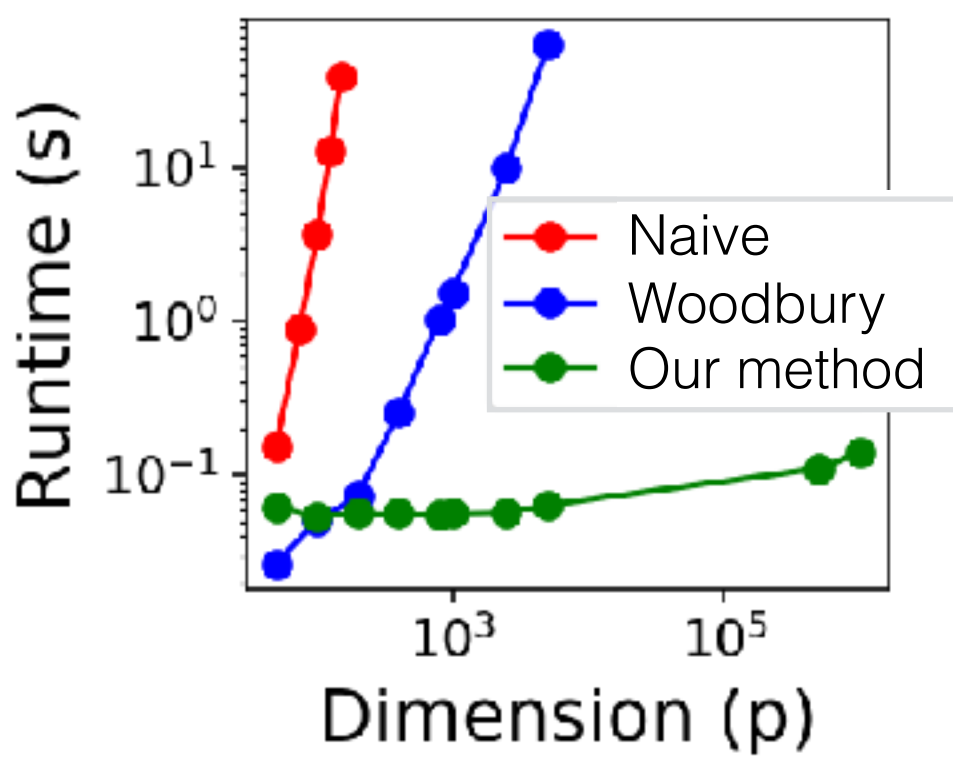

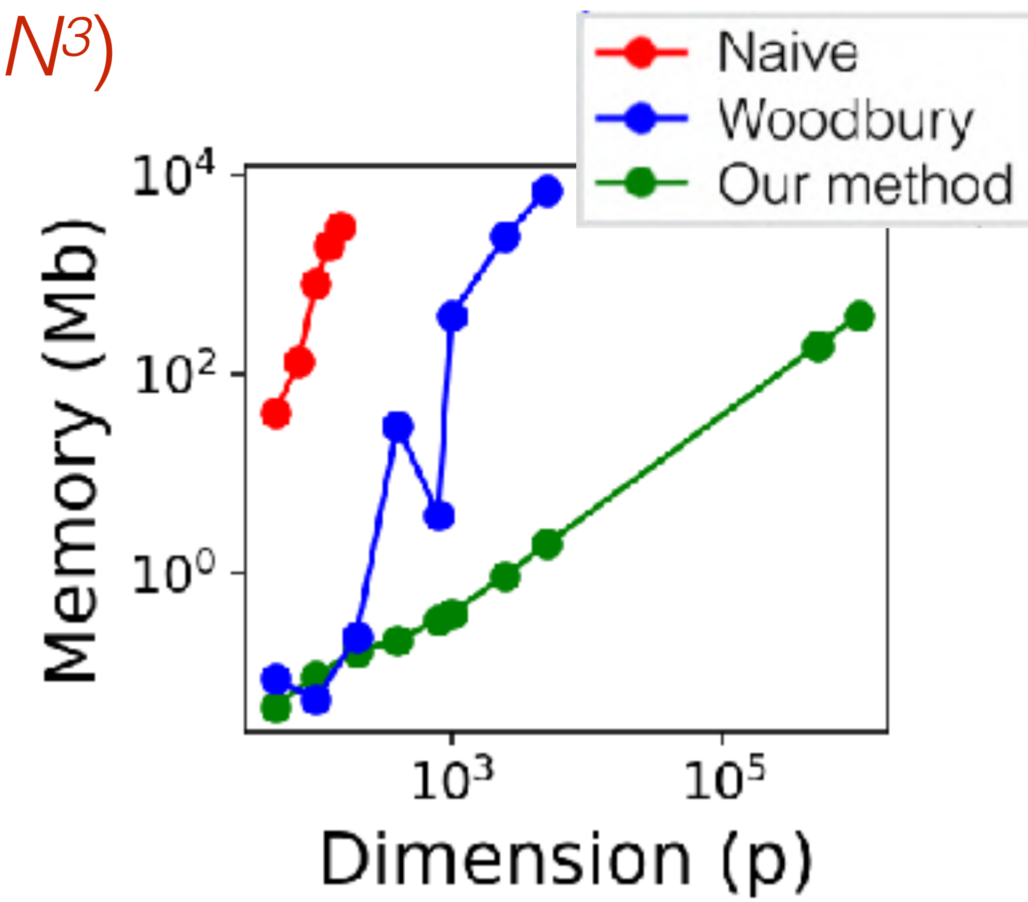

Kernel Interaction Sampler vs. Naive MCMC

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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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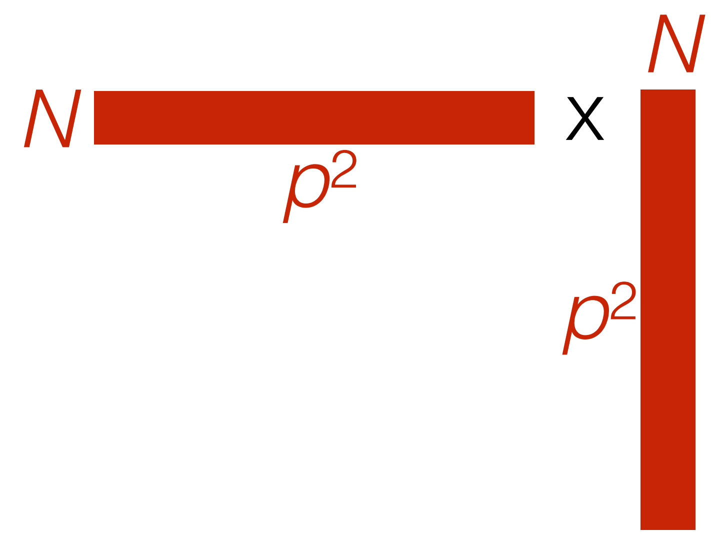

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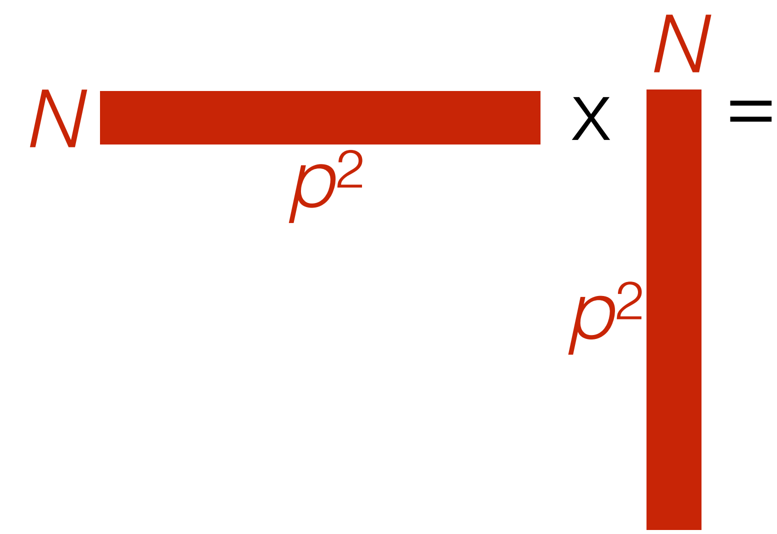

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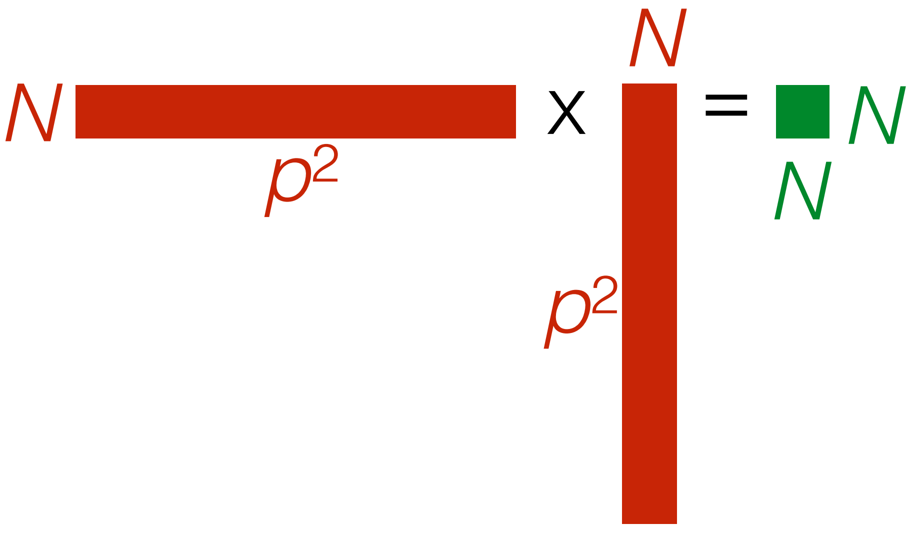

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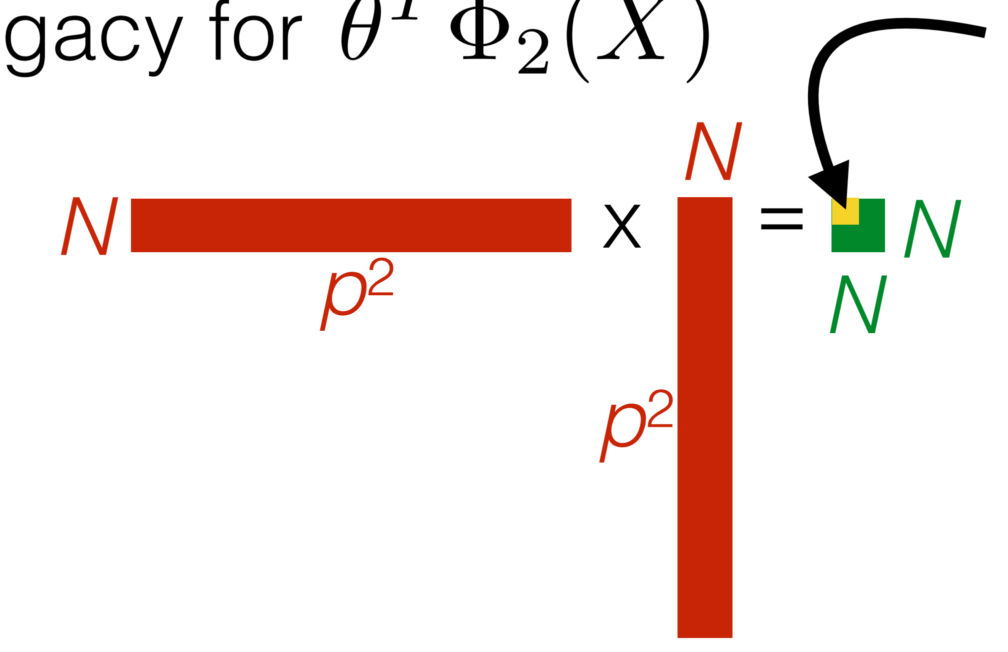

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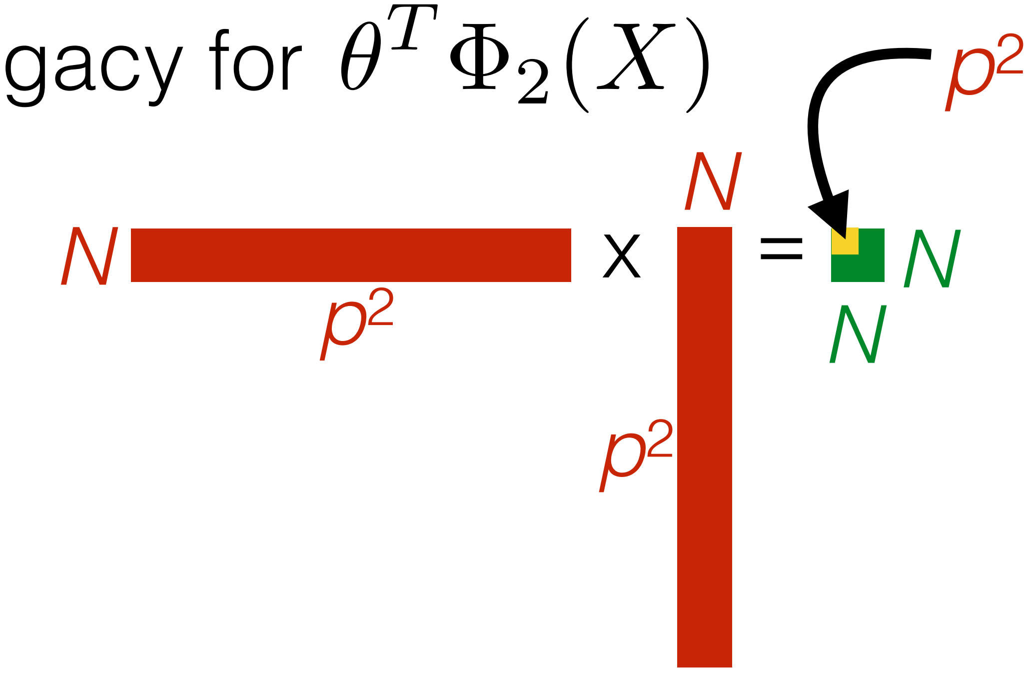

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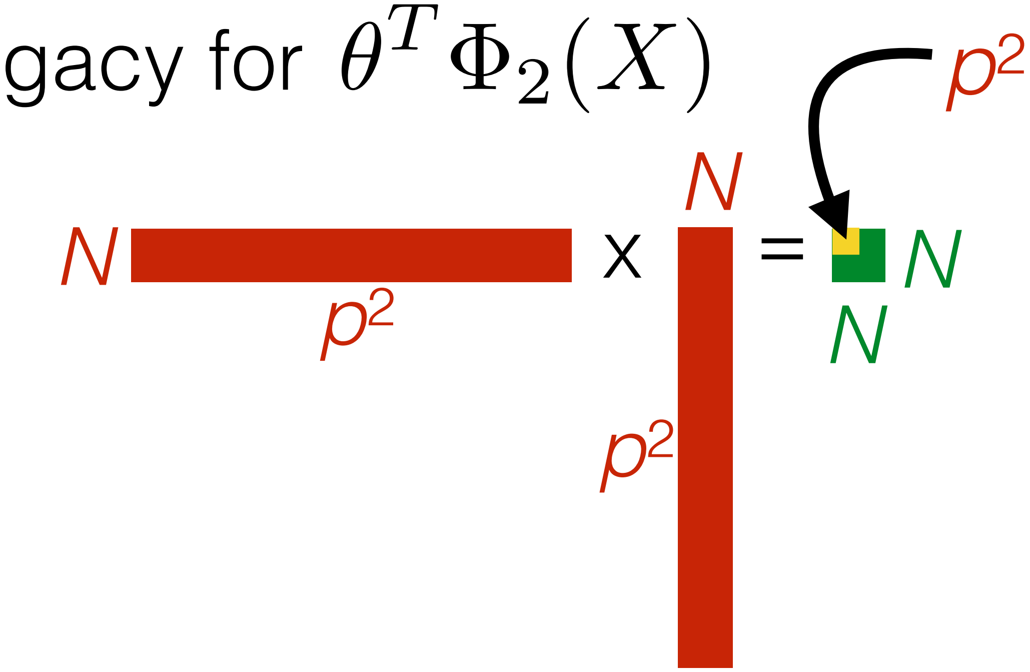

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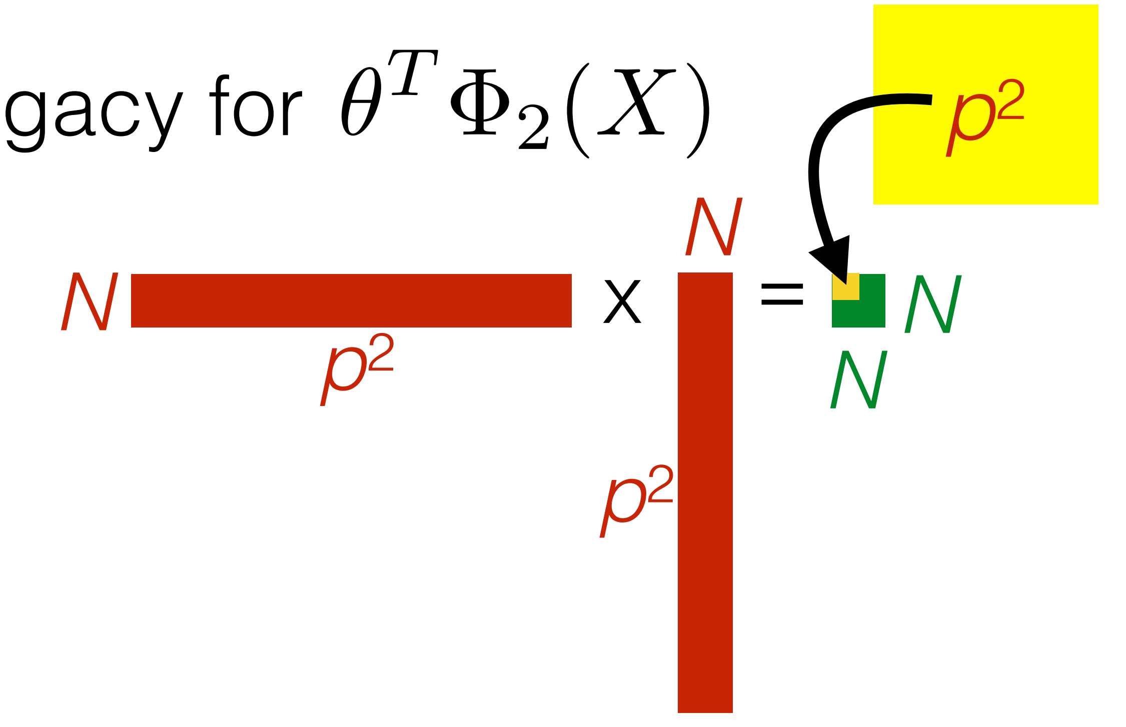

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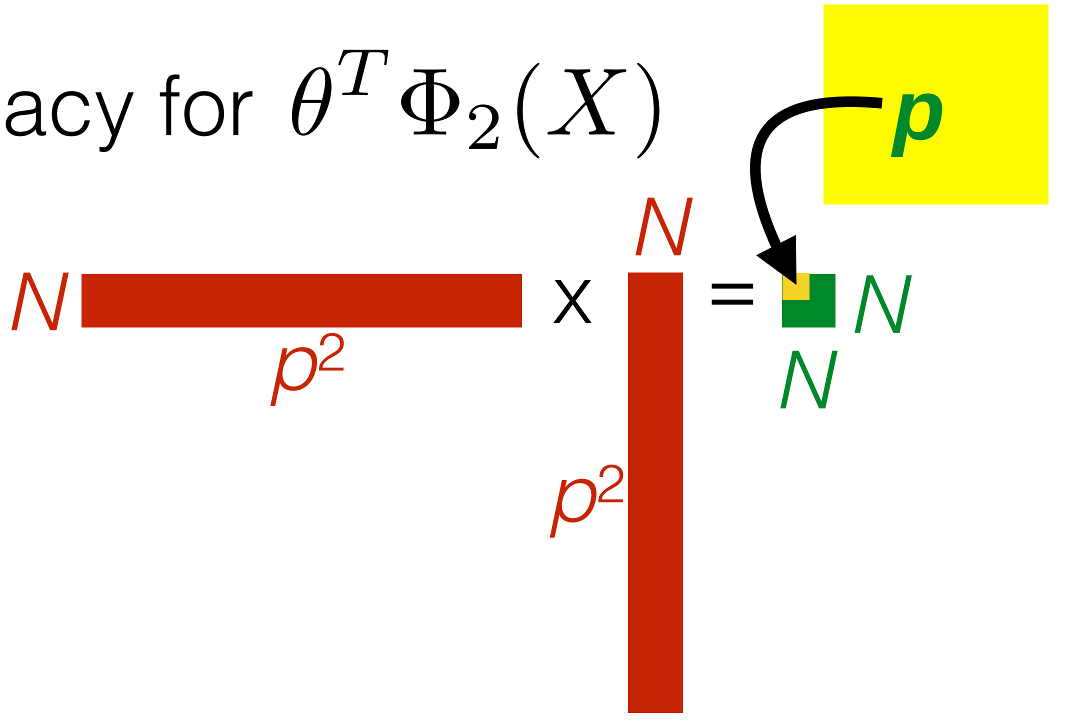

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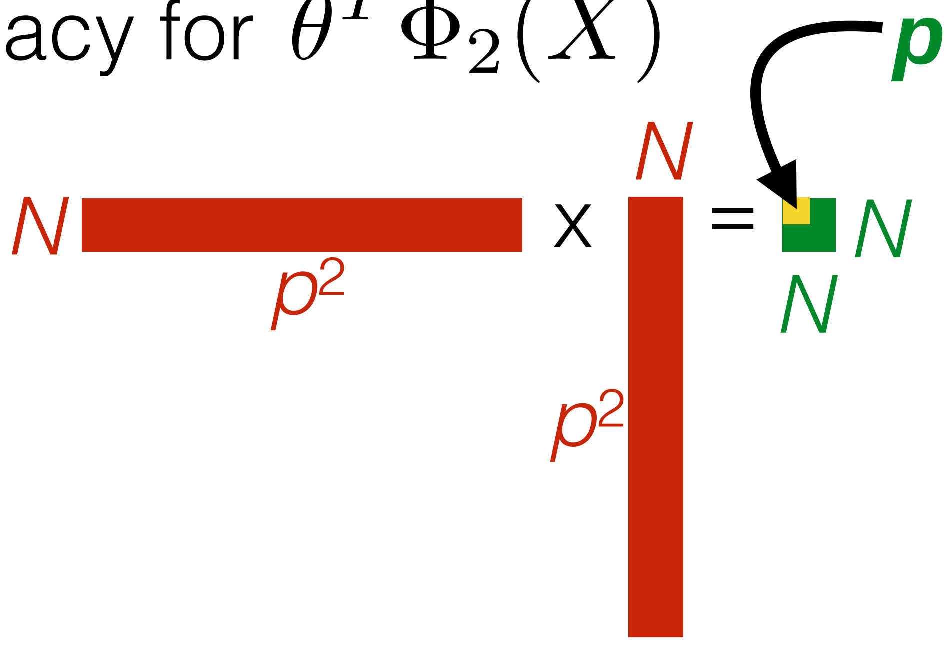

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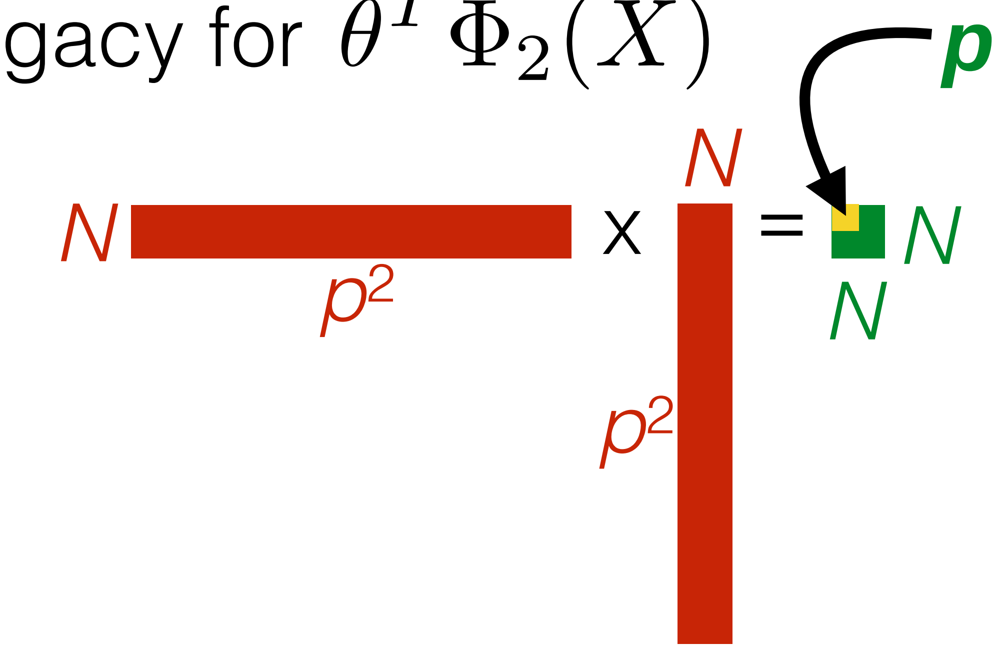

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Roadmap

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- Our method
  - A Bayesian generative model
  - Fast inference (using Gaussian processes)
  - Fast reporting of results
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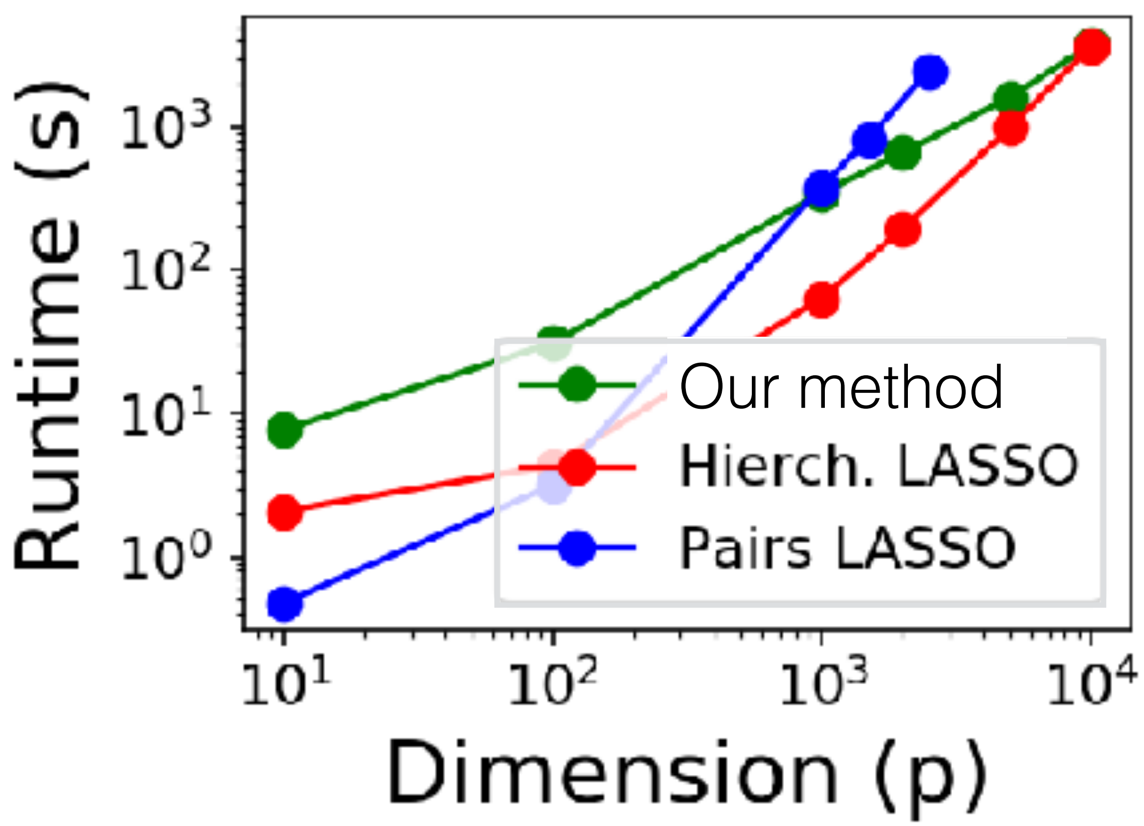

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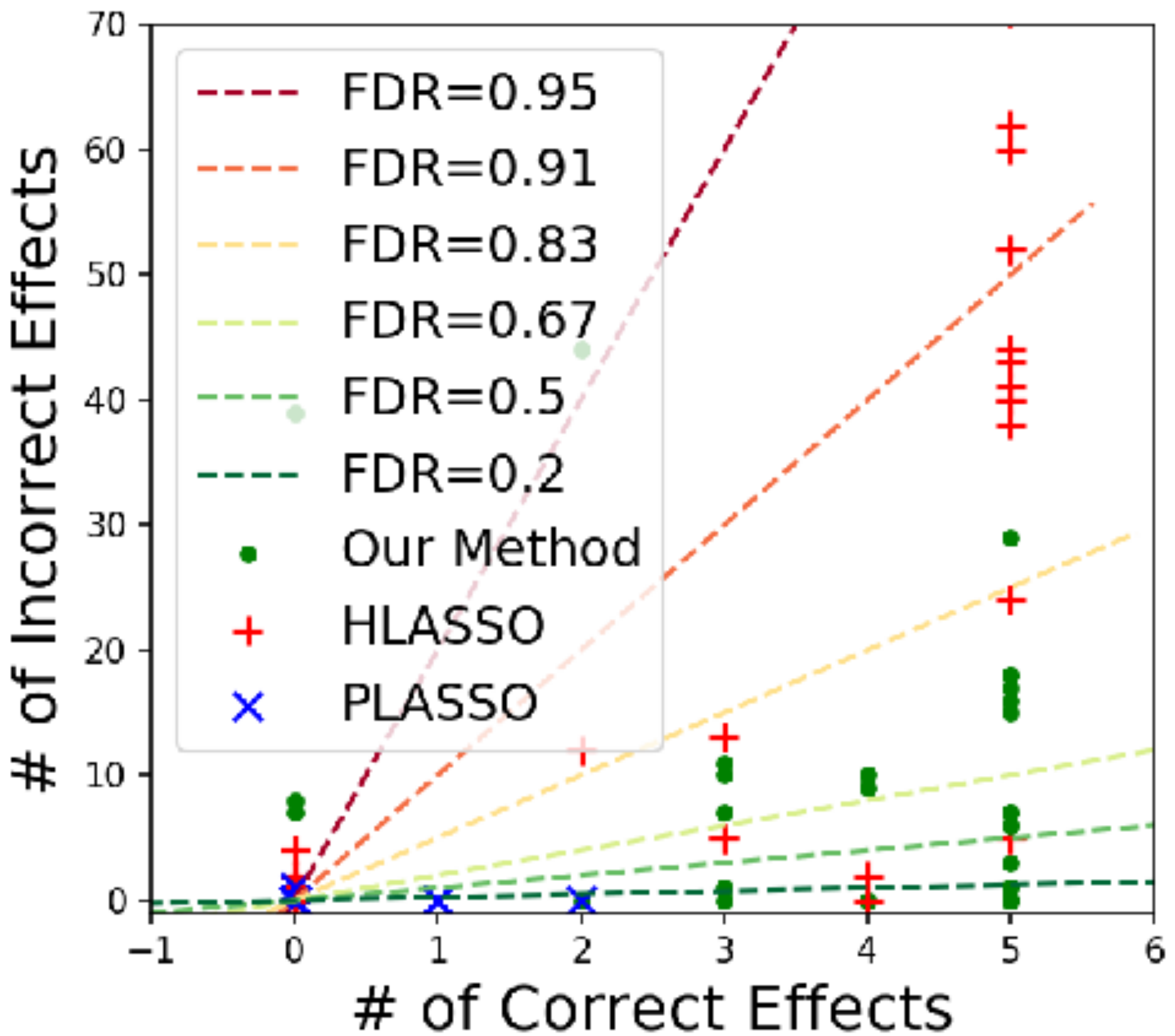

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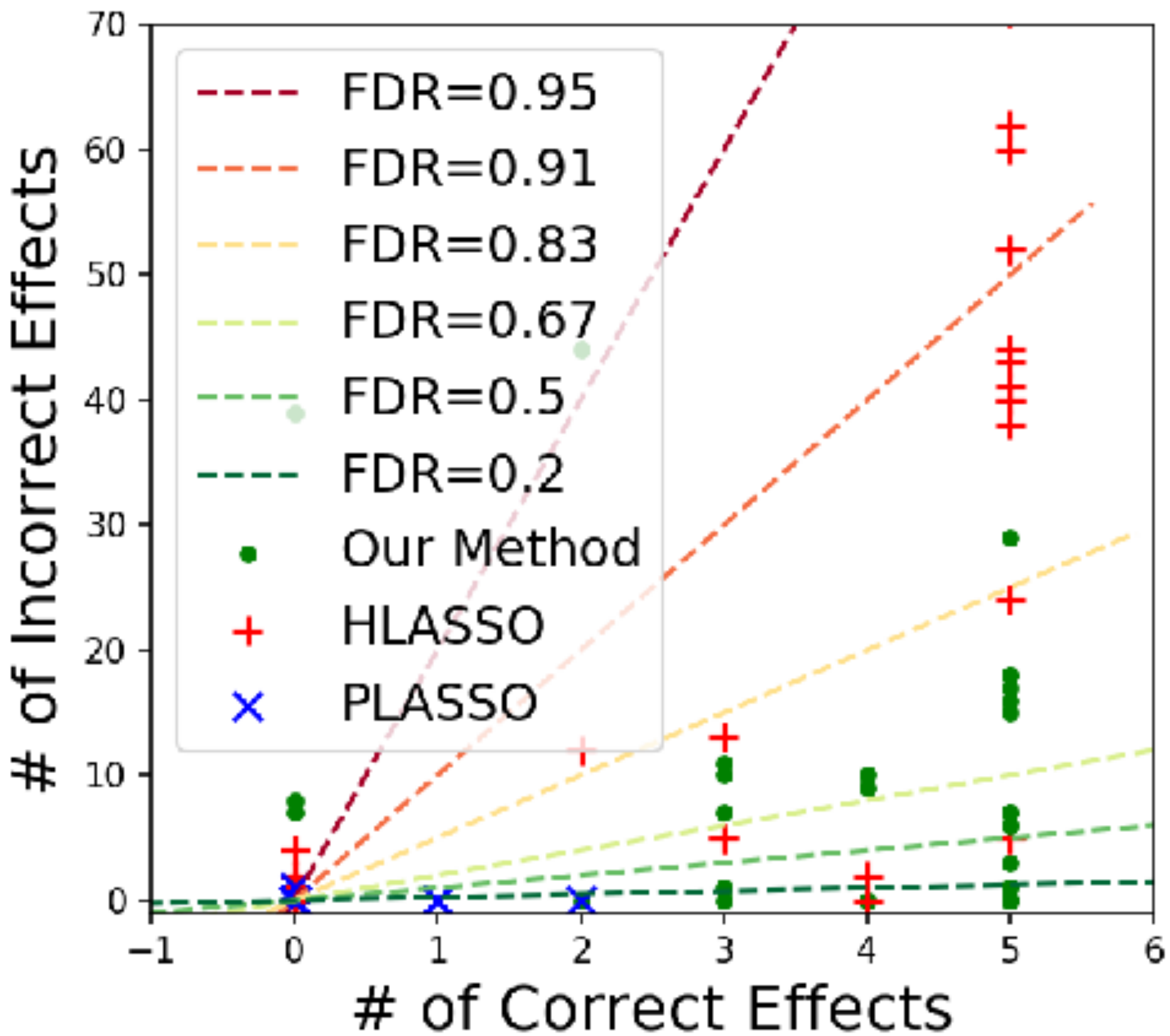
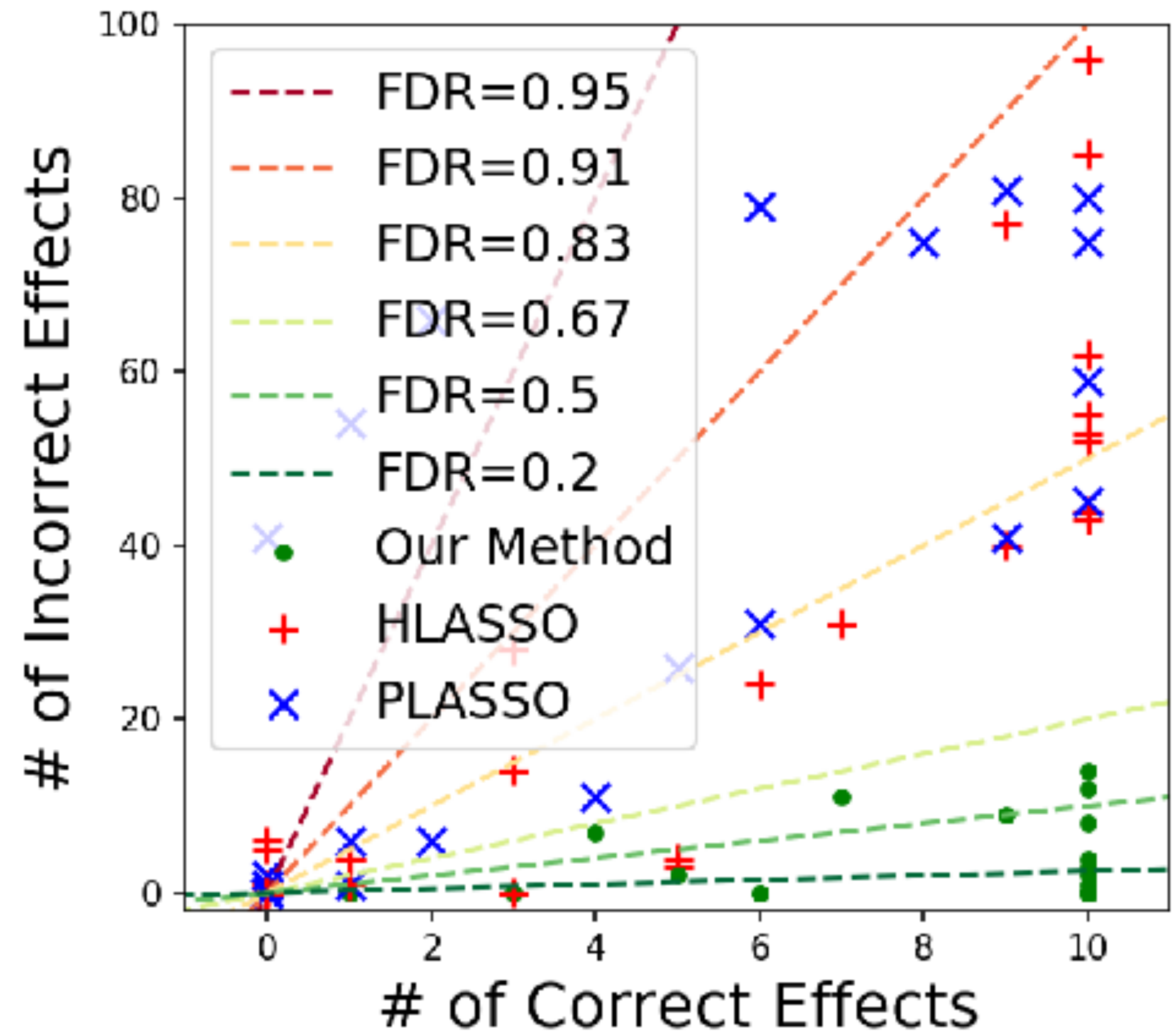


Pairwise effects



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- Augment p with 200 fake (noise) covariates
    - 21,321 total parameters

Experiments: Real data

- Covariates and response: Auto MPG
- $N = 398$, $p = 6$ (real-valued), but…
- Augment p with 200 fake (noise) covariates
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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

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Up next: (1) Nonlinearity; (2) Remove strong hierarchy assumption

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WT Stephenson, S Ghosh, TD Nguyen, M Yurochkin, SK Deshpande, and T Broderick. Measuring the sensitivity of Gaussian processes to kernel choice. *AISTATS* 2022, to appear.