Fast Discovery of Pairwise Interactions in High Dimensions using Bayes

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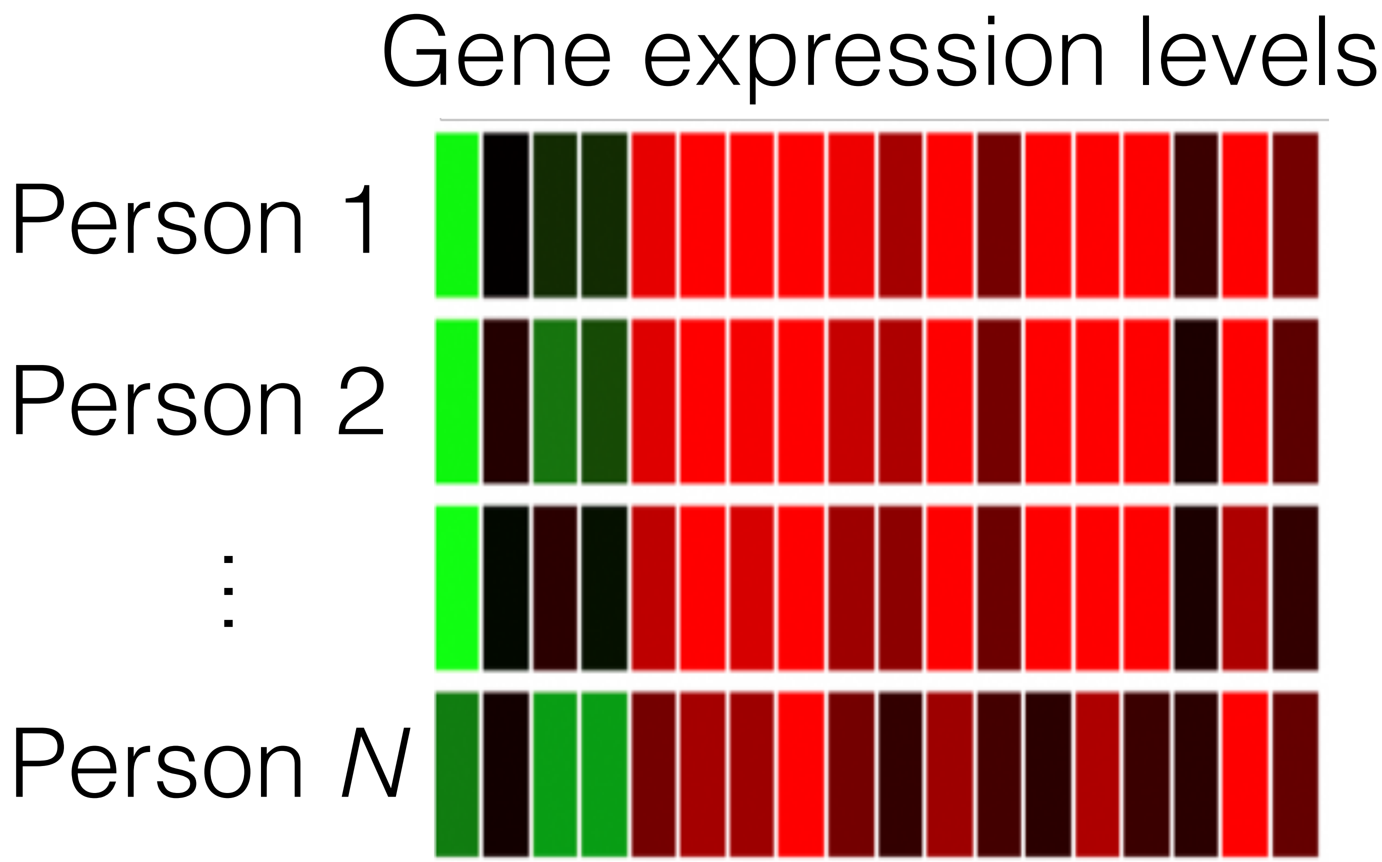
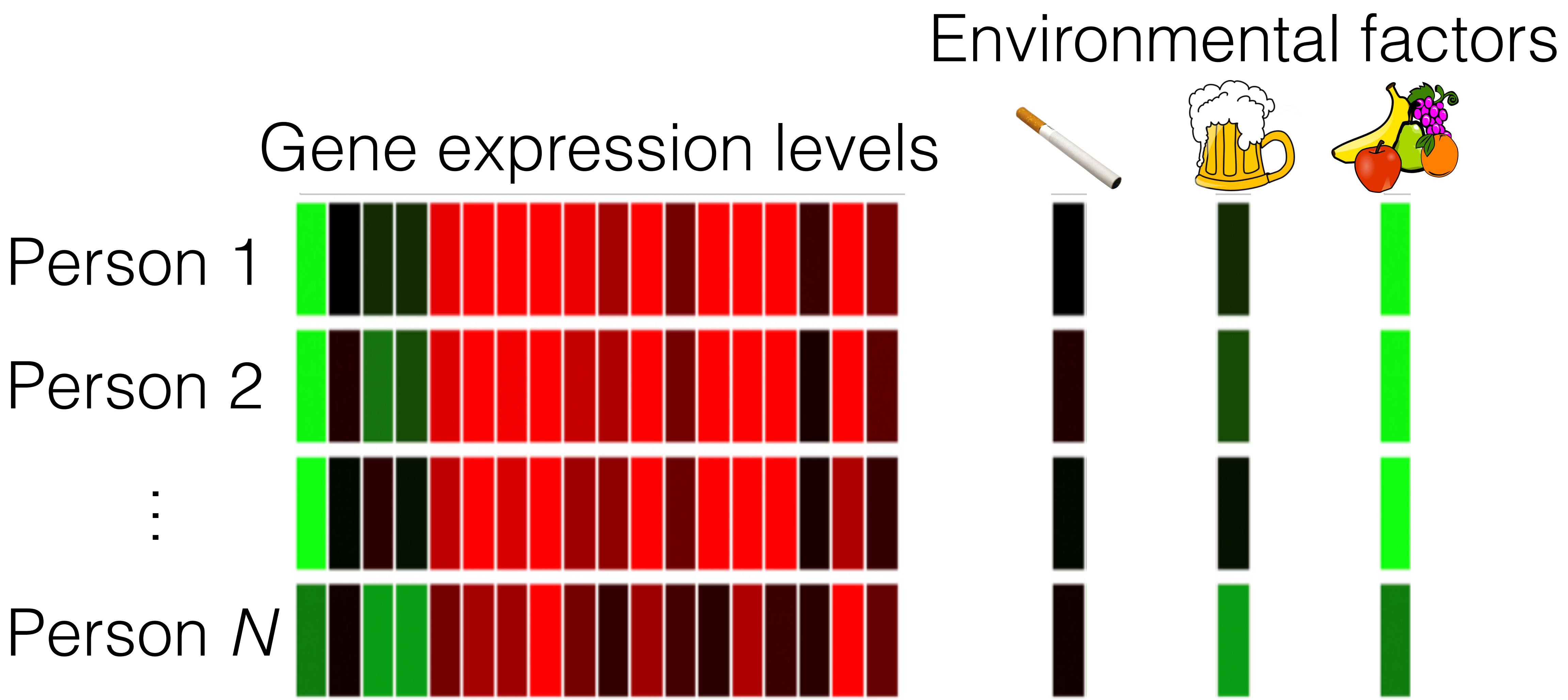
EECS, MIT

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


Gene expression levels
Person 1
Person 2
⋮
Person N


Environmental factors
Gene expression levels
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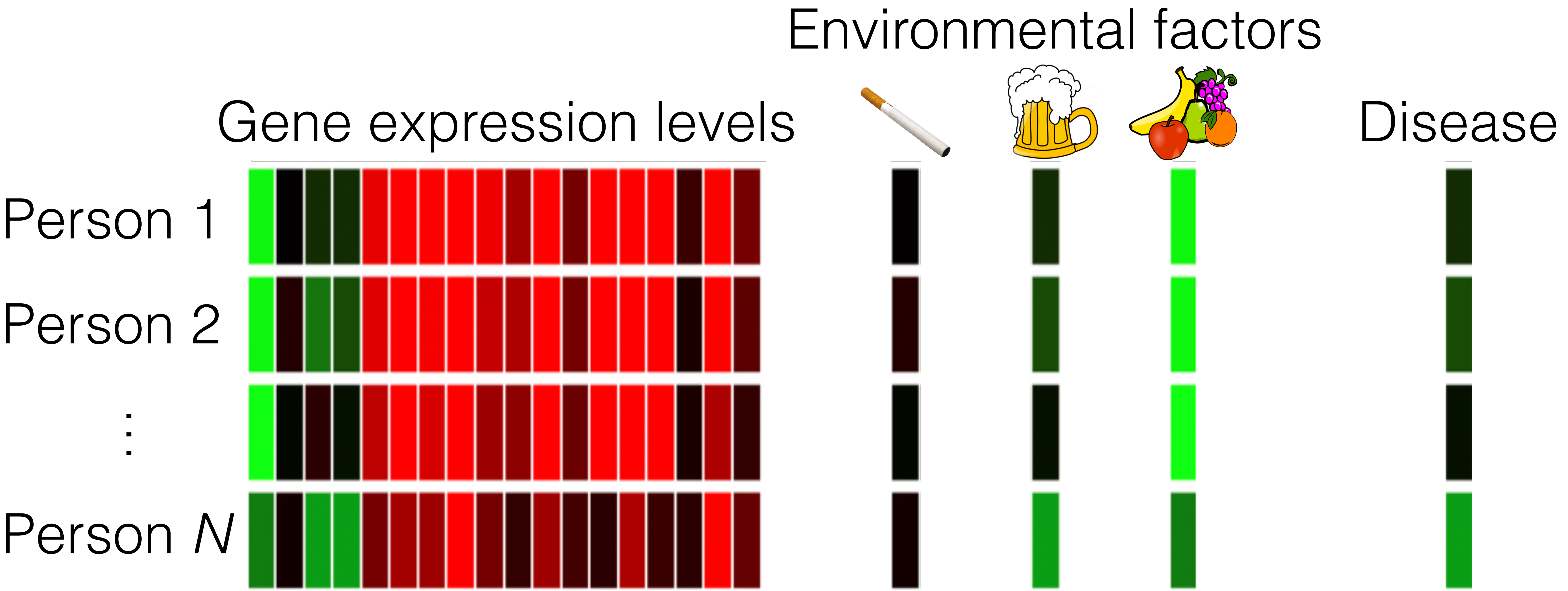
Environmental factors
Gene expression levels
Disease
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Person 2
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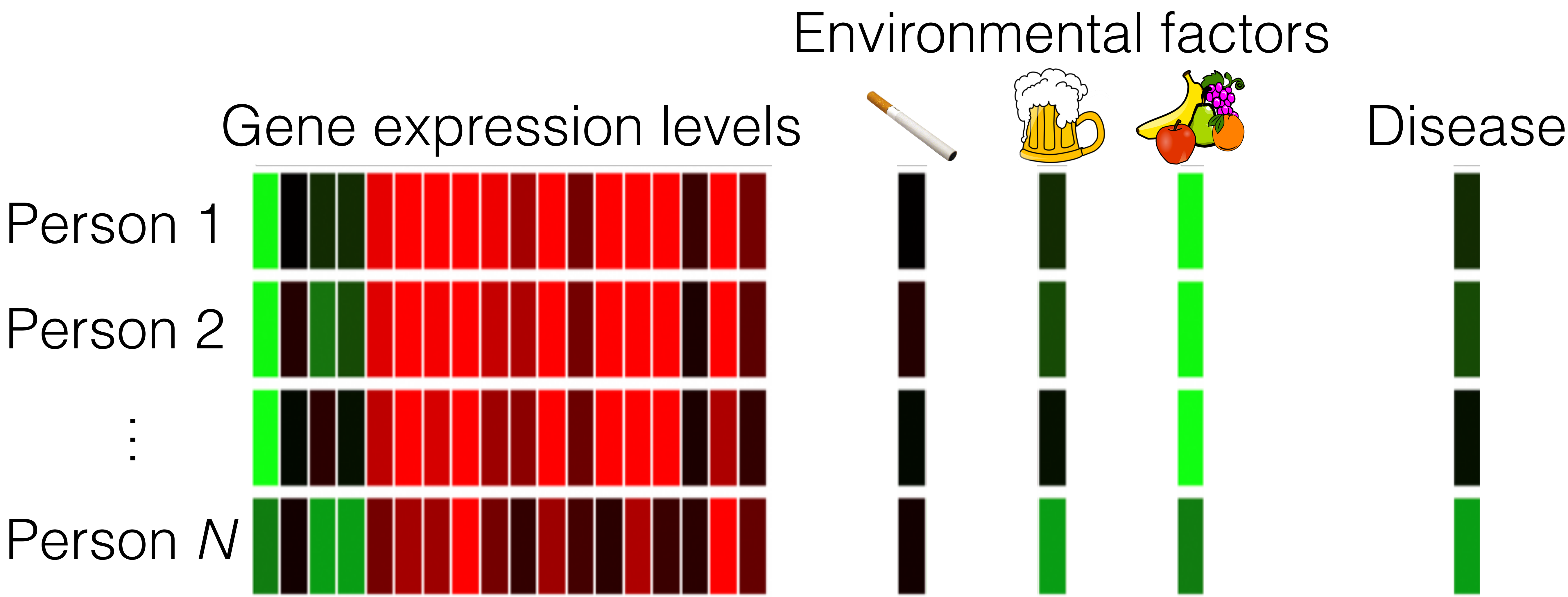
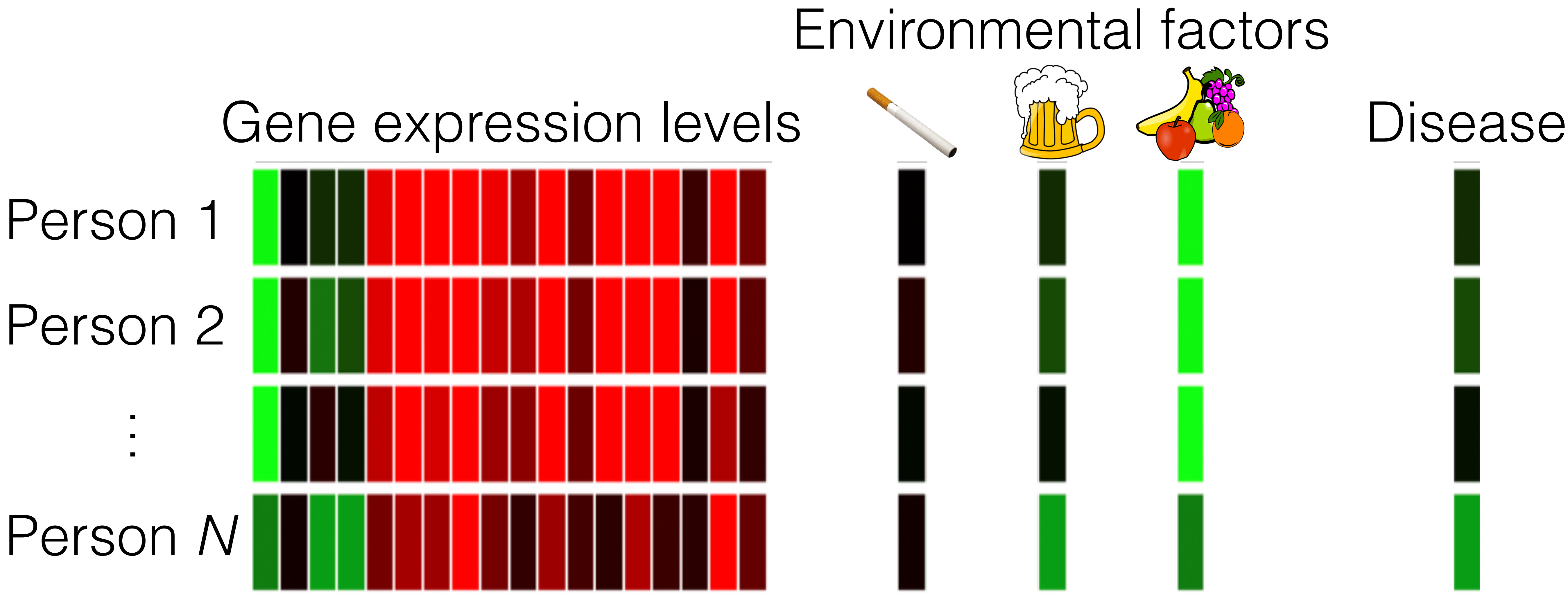


- Which genes/factors are associated with a disease?



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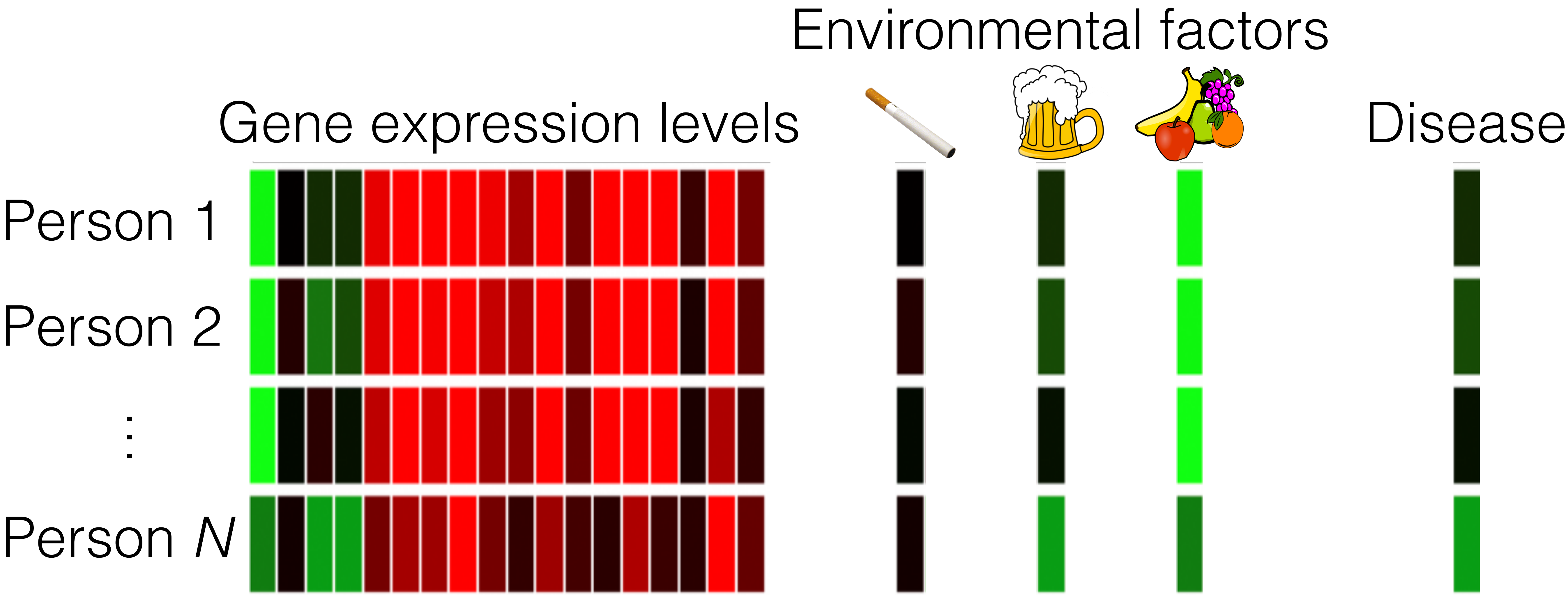

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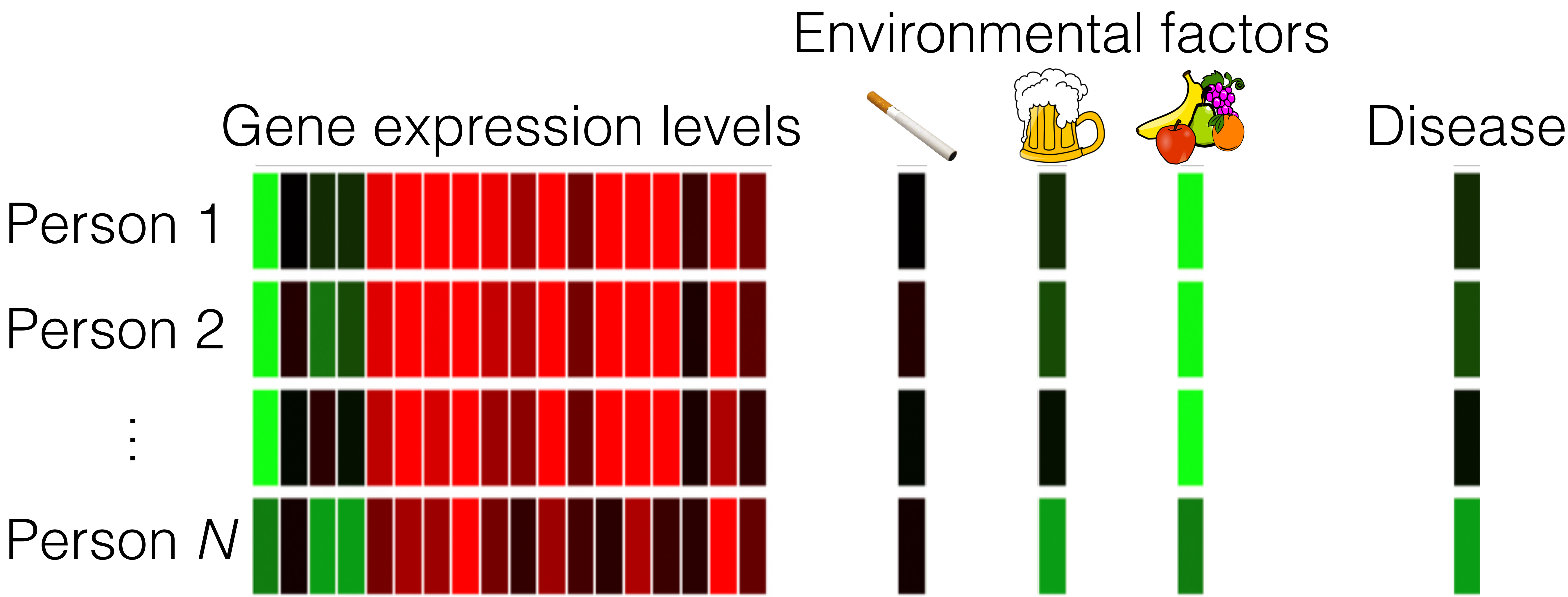

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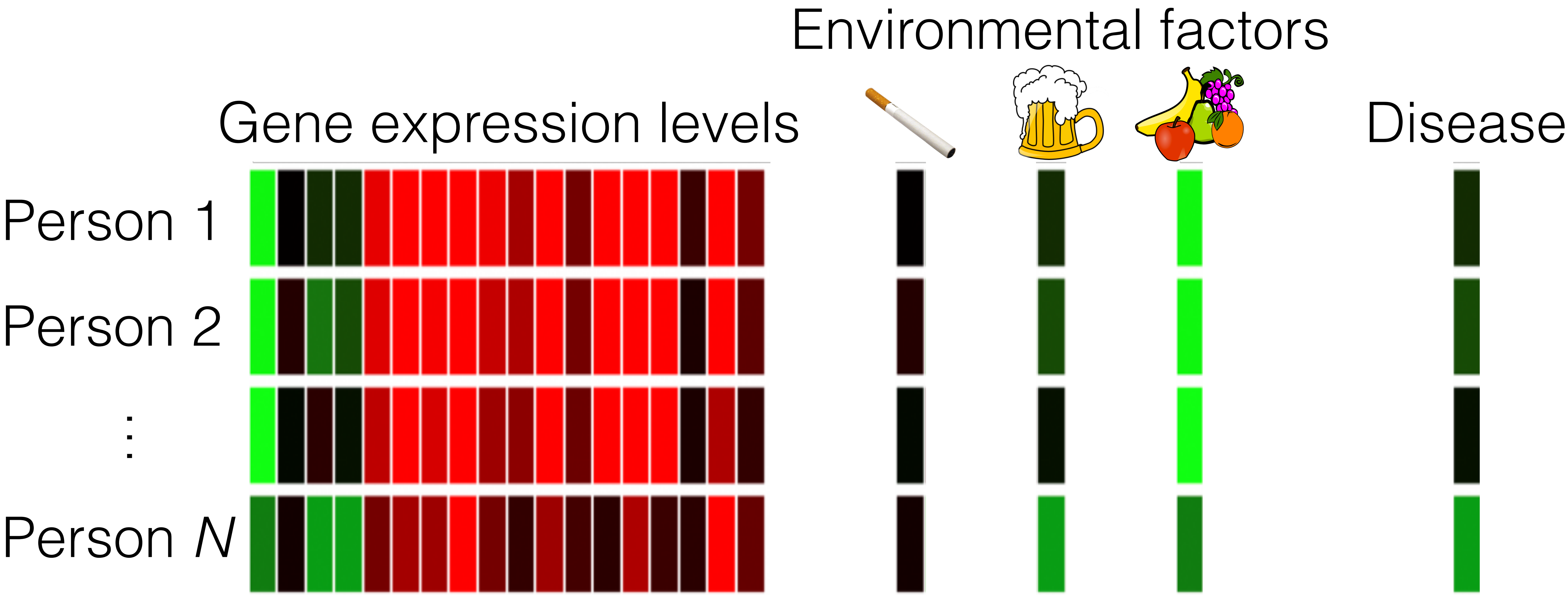

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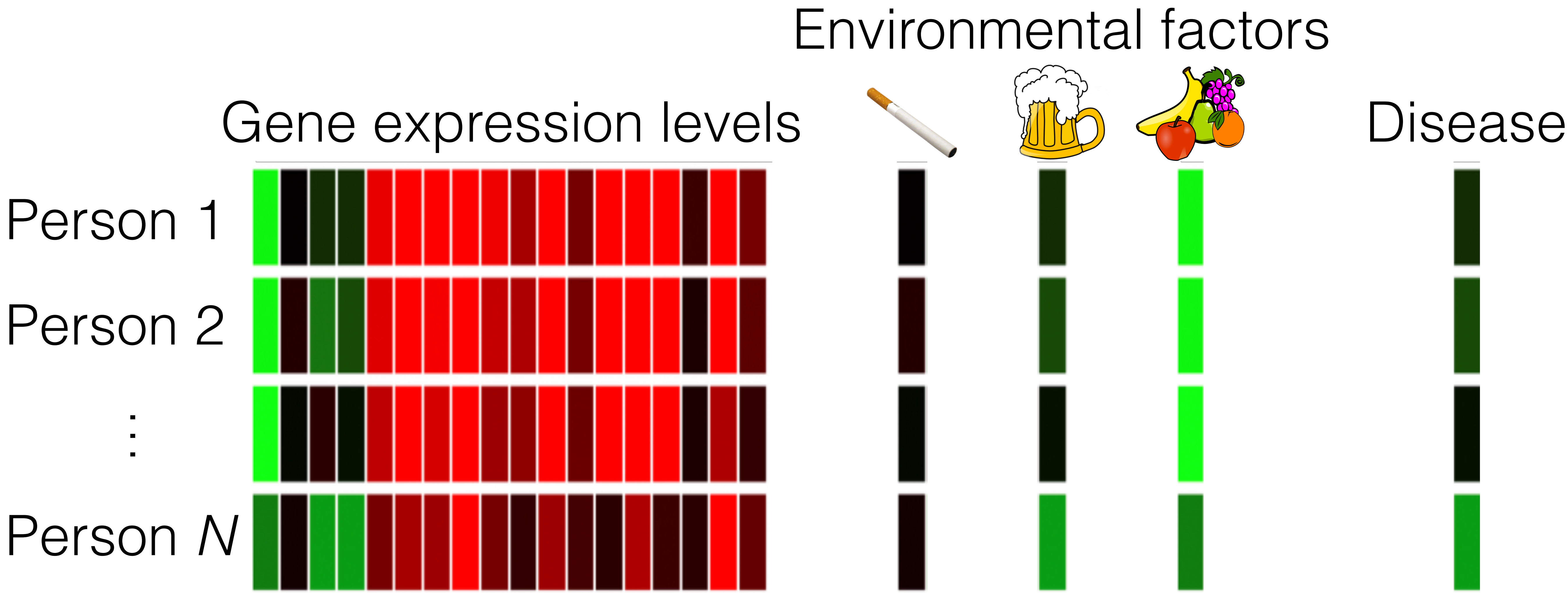
Pairwise interactions in high dimensions



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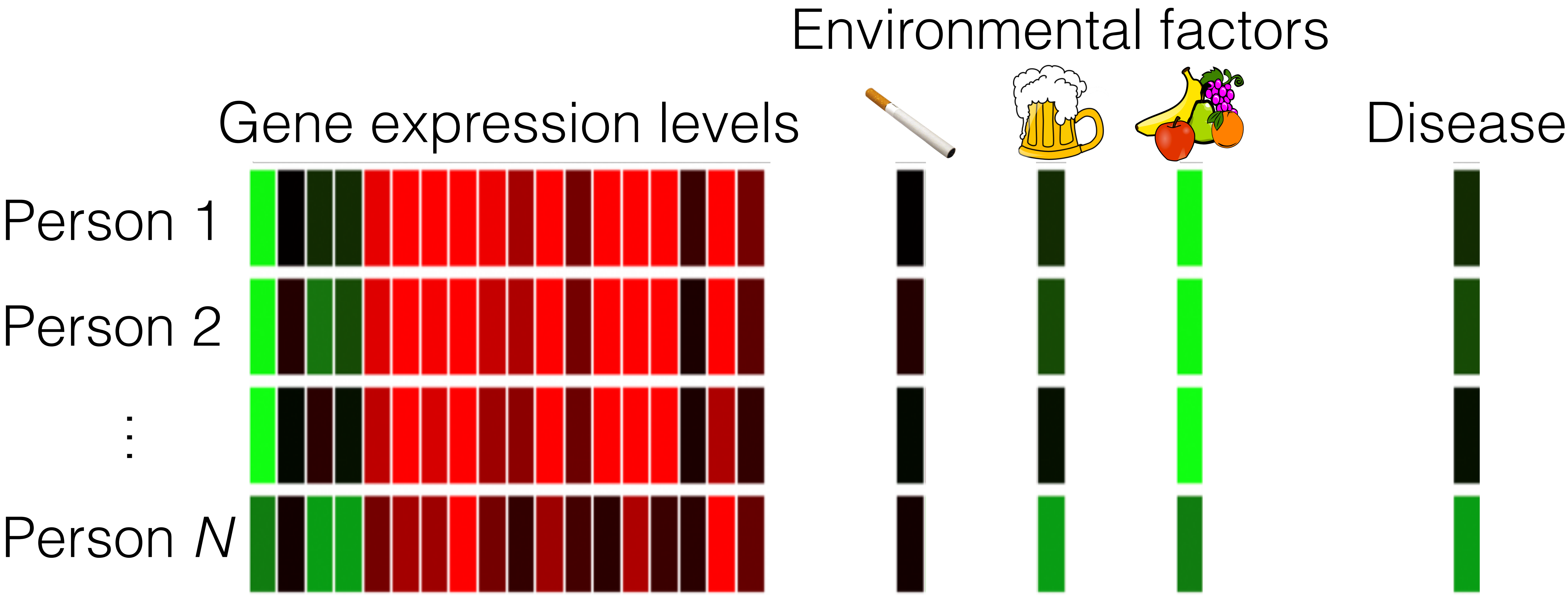

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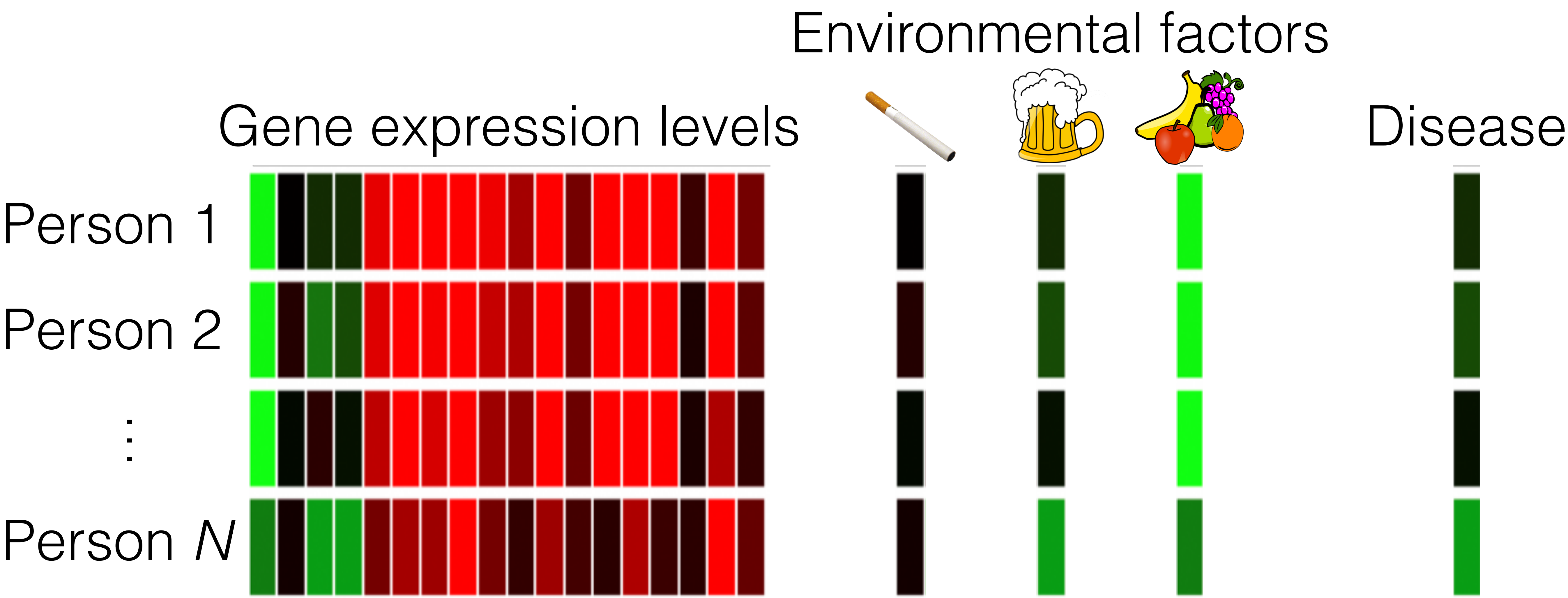

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- **We provide**: Fast, accurate (Bayes) method for interaction discovery
    - Better scaling in p & better accuracy than LASSO-based methods. Orders of magnitude faster than naive Bayesian inference

Roadmap

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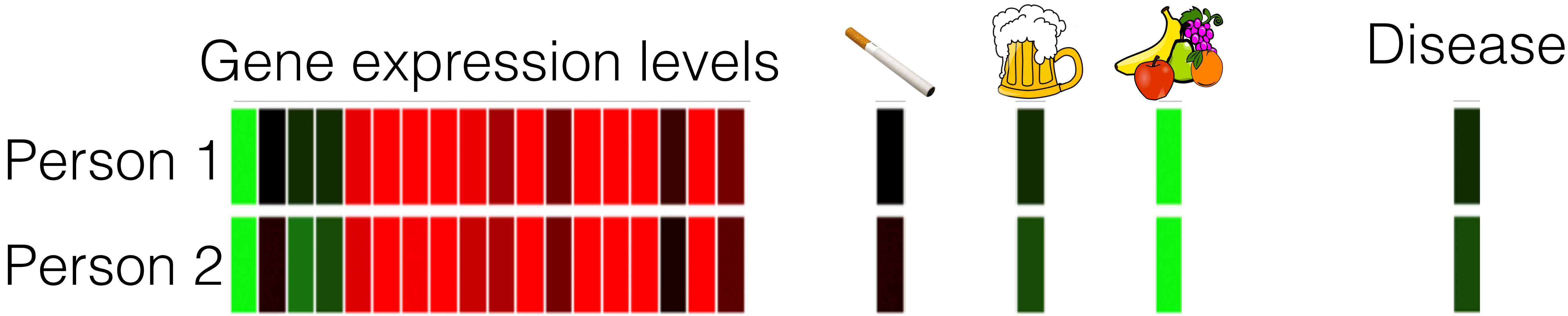
Discovering main and interaction effects



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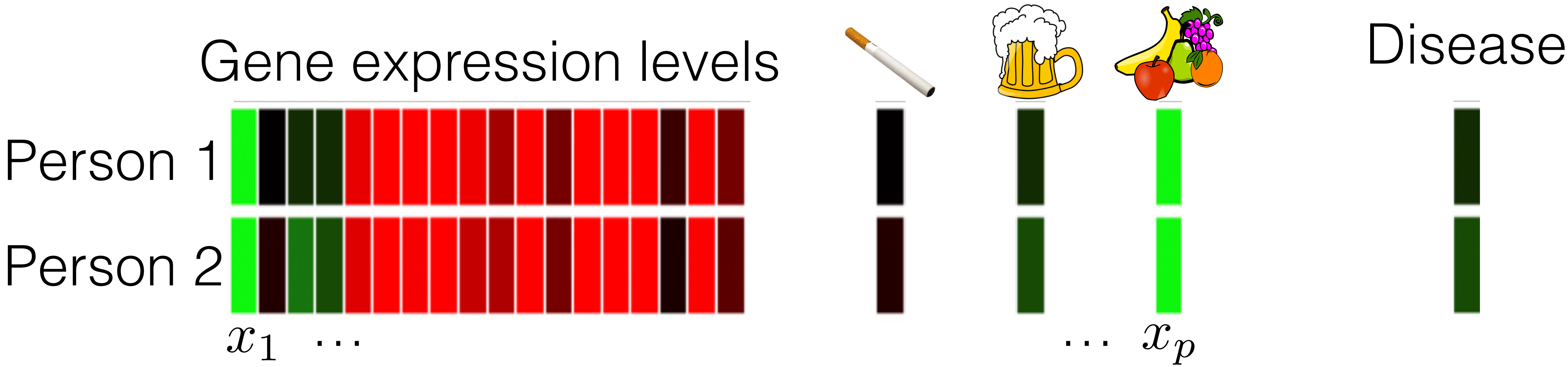

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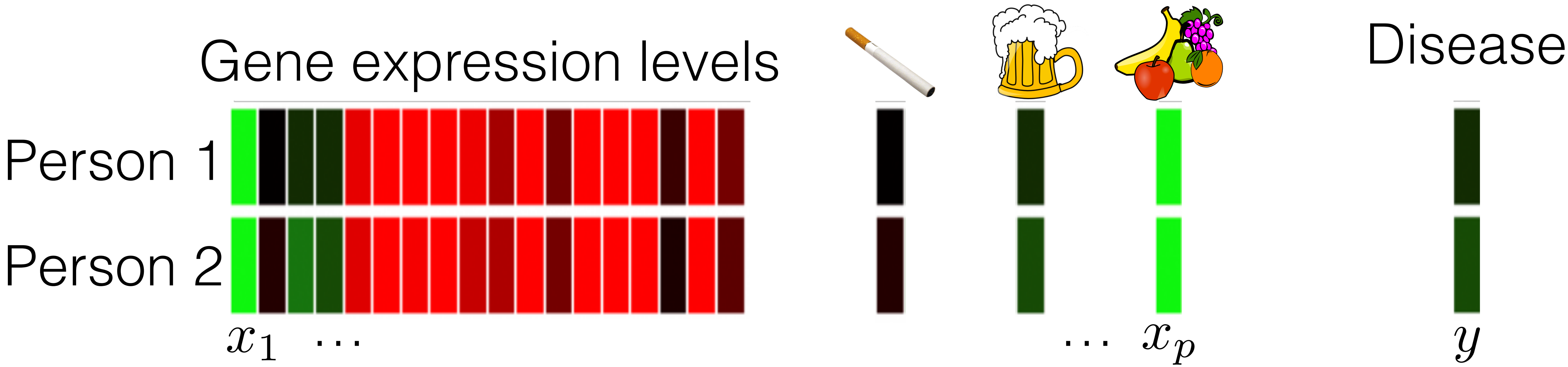

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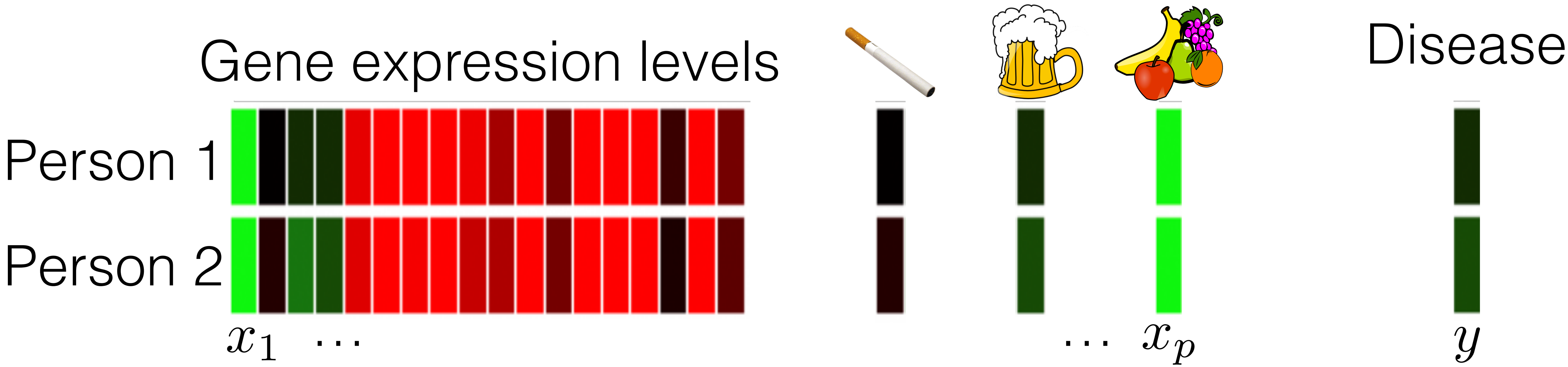

$$x^\top := [x_1, \ldots, x_p]$$

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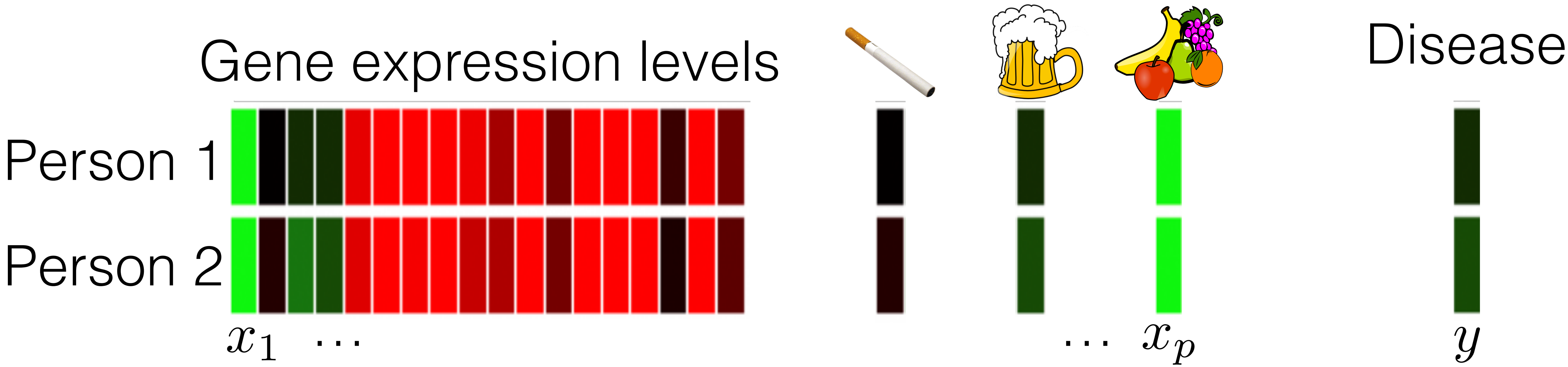

$$x^\top := [x_1, \ldots, x_p]$$

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

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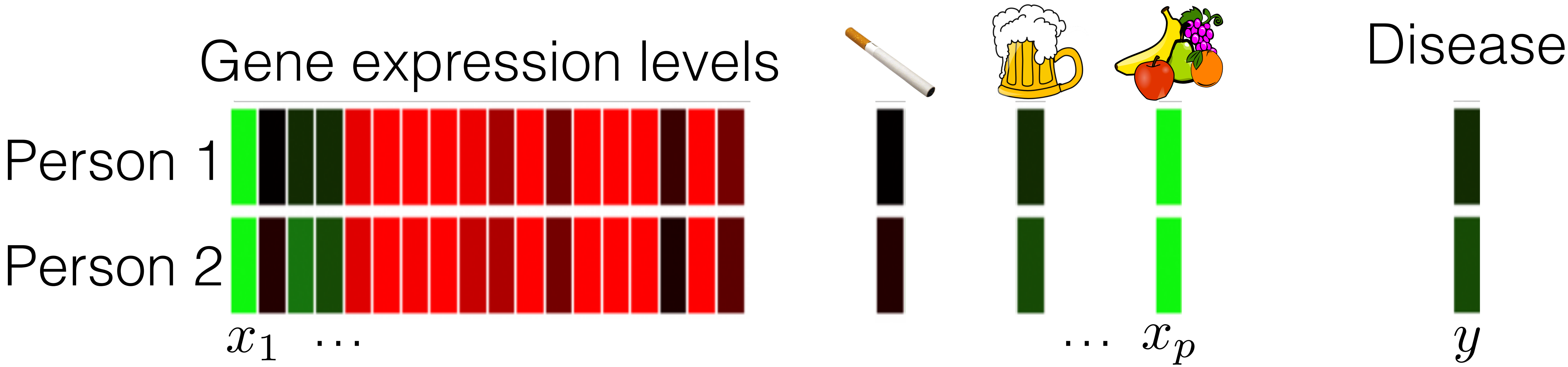

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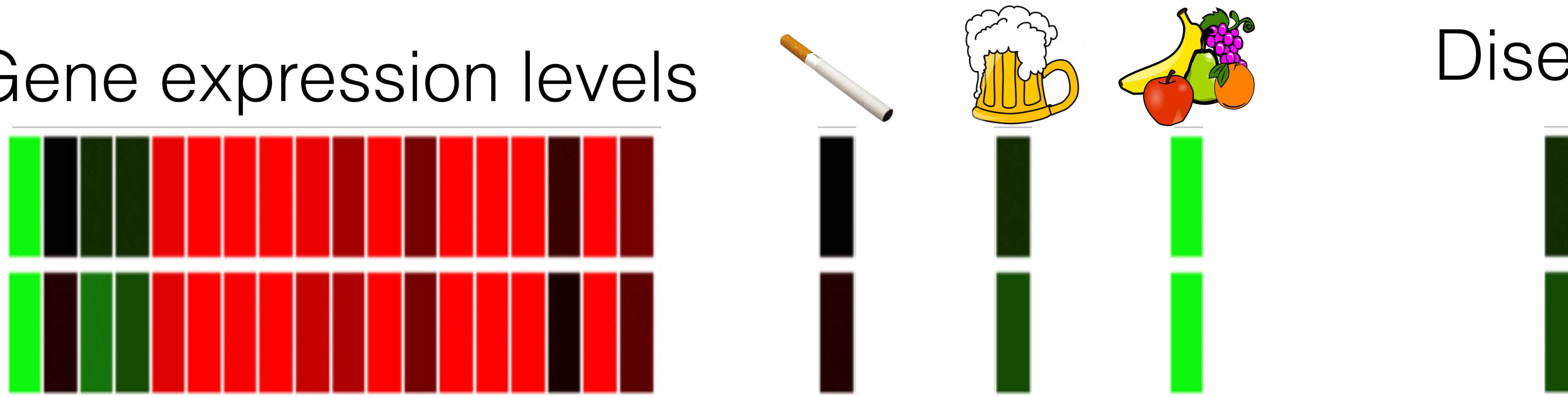

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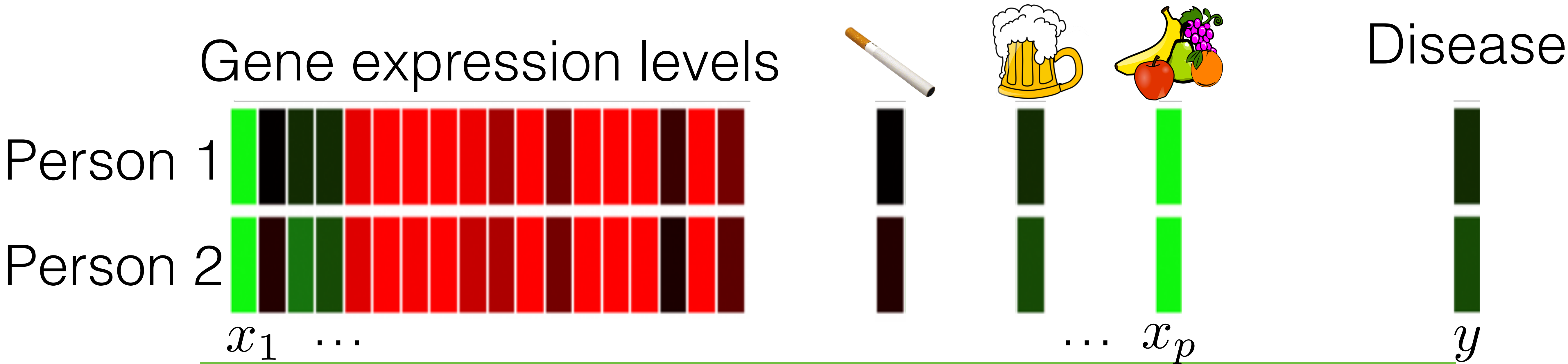

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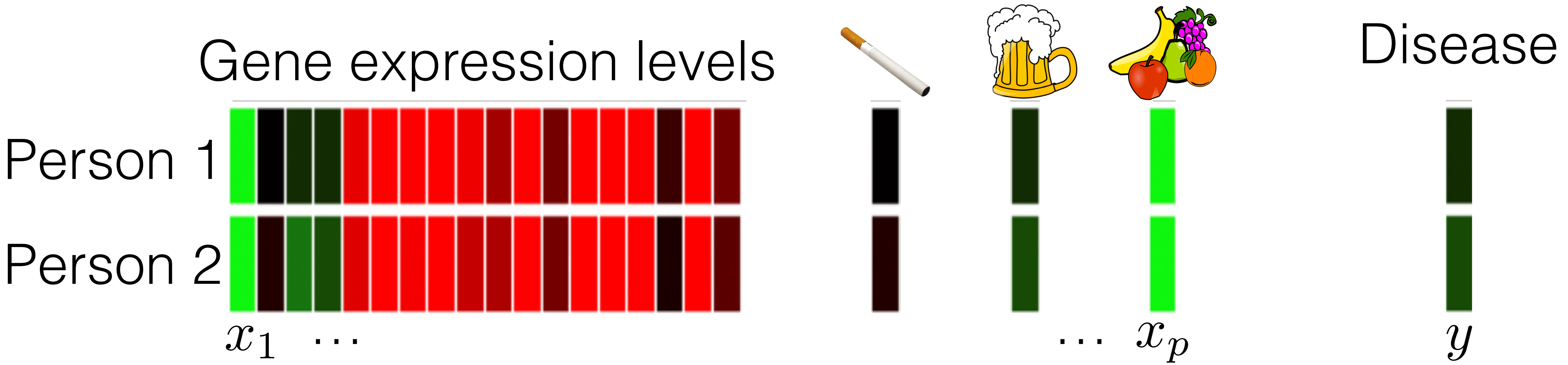

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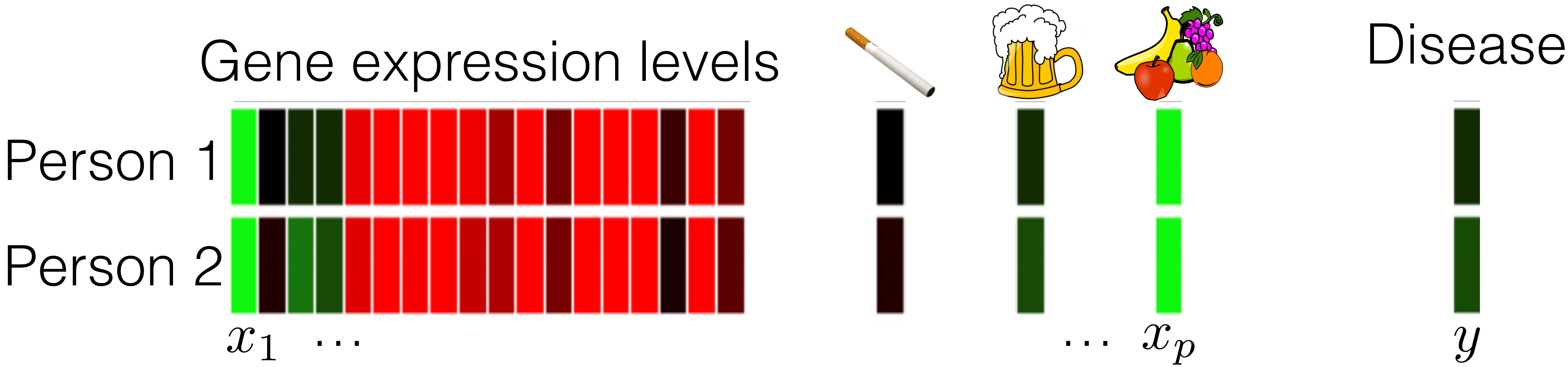

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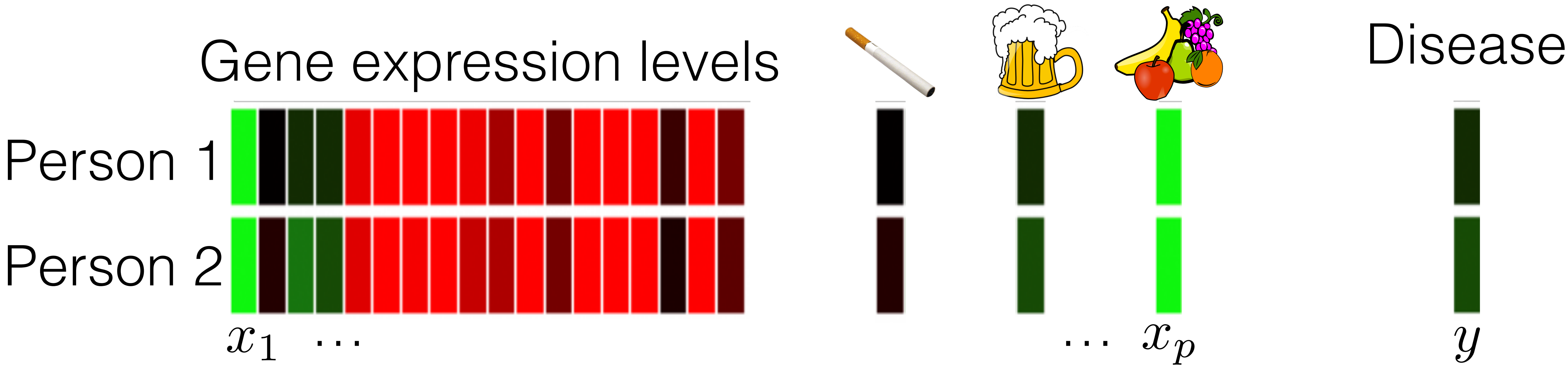

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Discovering main and interaction effects

Gene expression levels

Disease

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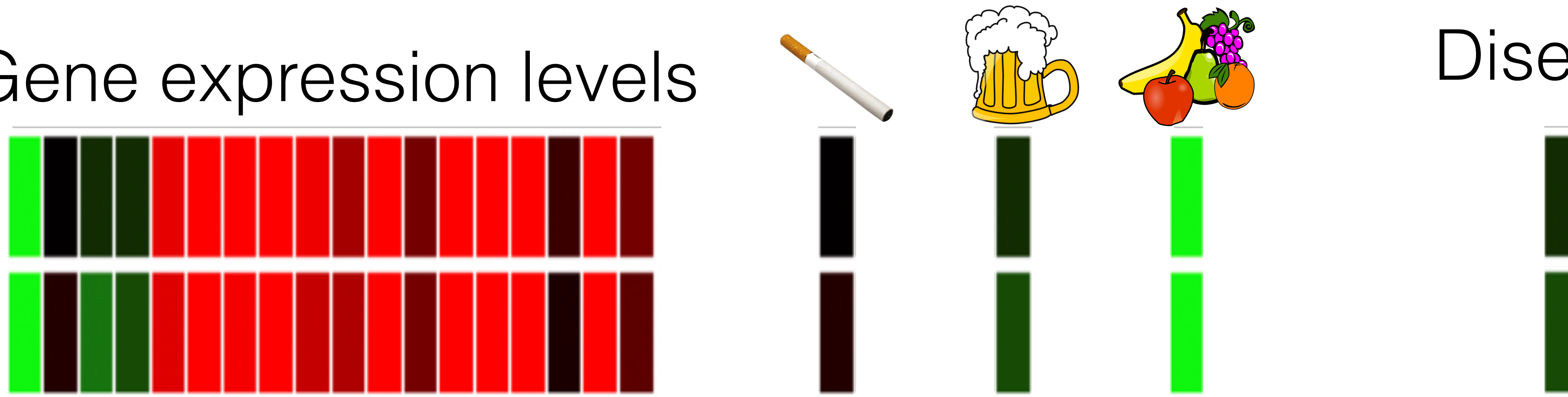

$x_1 \quad \cdots \quad\quad \cdots \quad x_p \quad\quad y$

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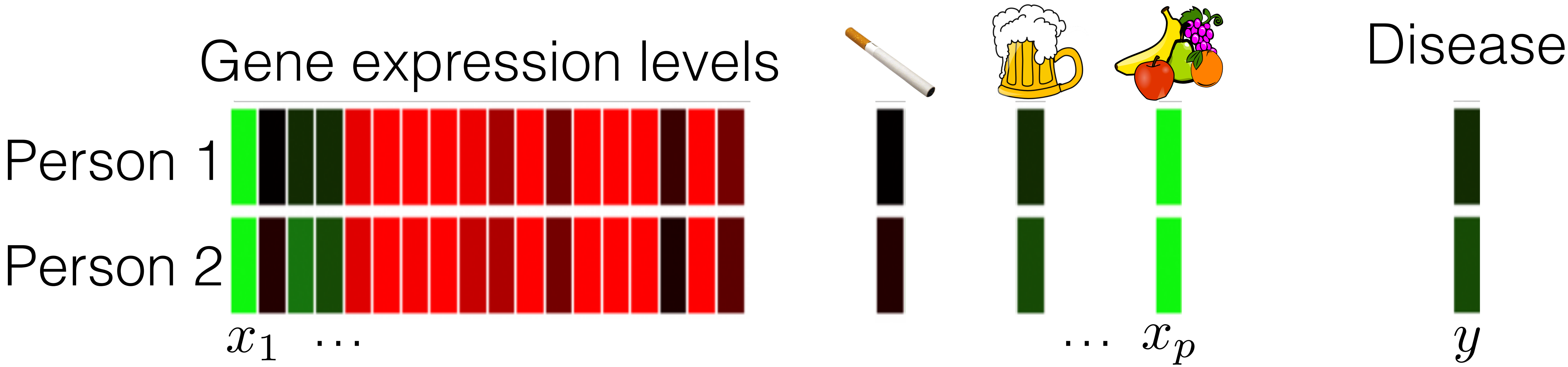

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- **Goal**: Parameter selection/estimation under assumptions:

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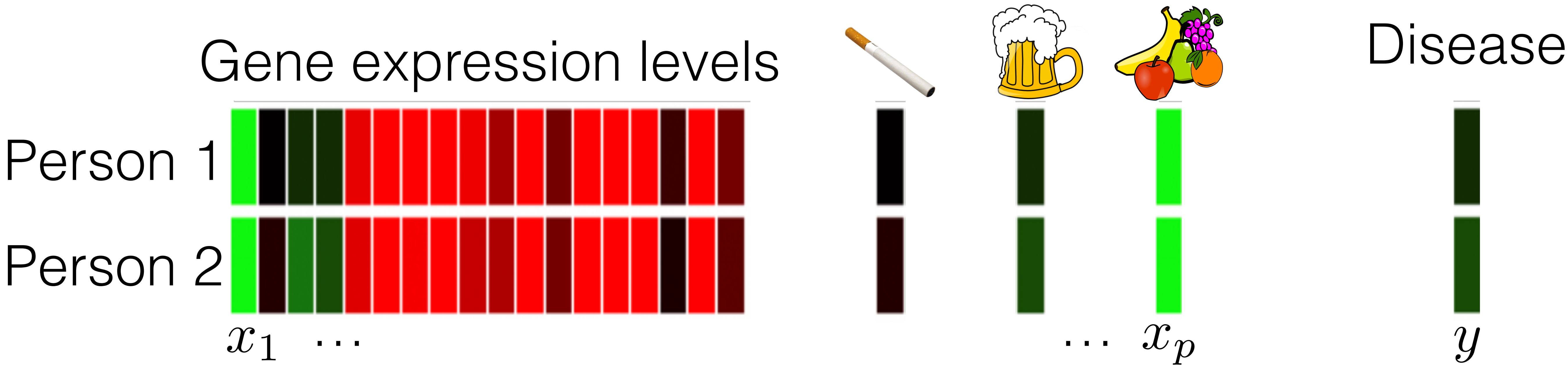

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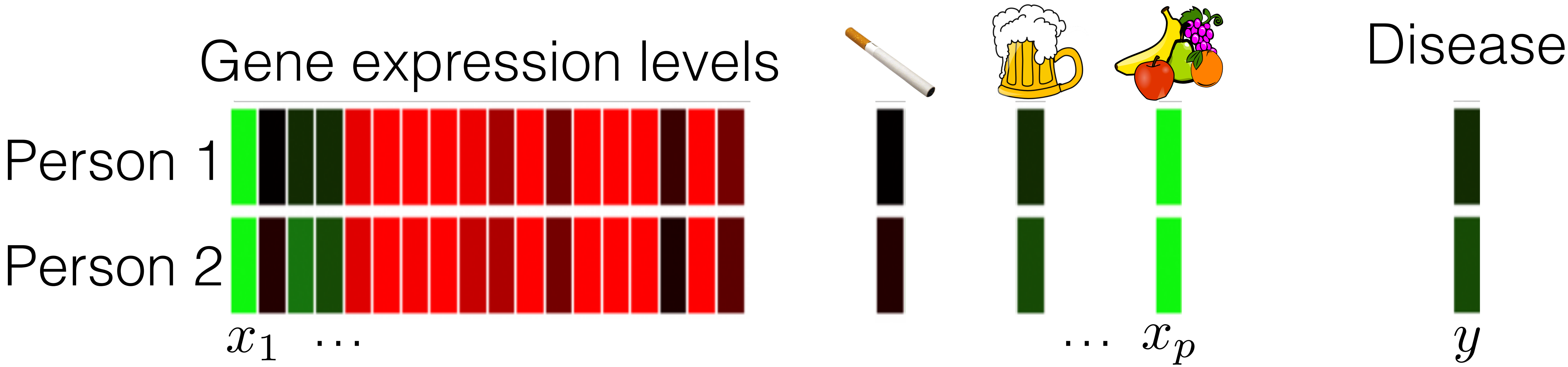

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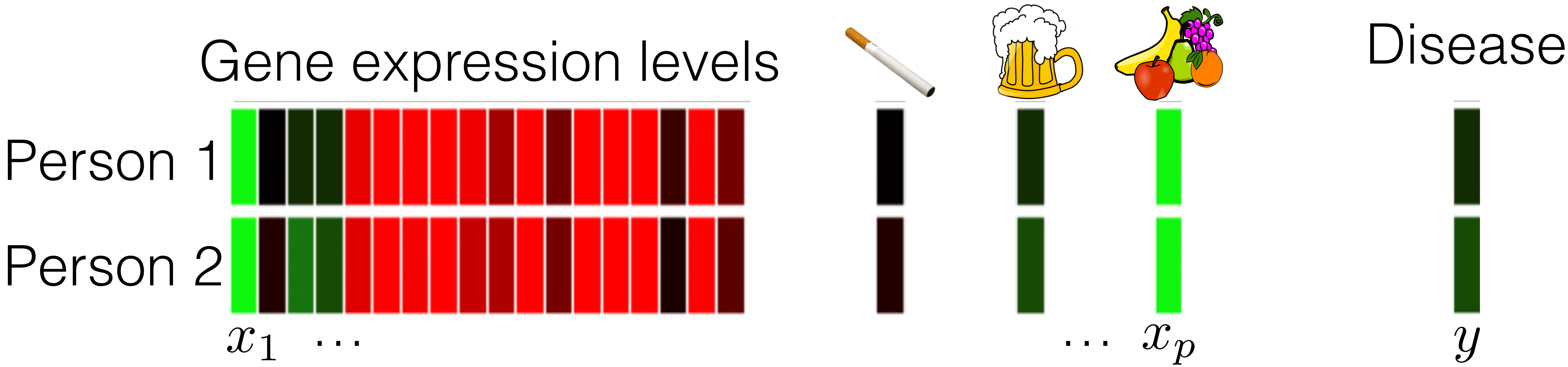
[Chipman 1996; Wu et al 2009; Bien et al 2013; Lim, Hastie 2015; Nakagawa et al 2016; Griffin, Brown 2017]

Discovering main and interaction effects



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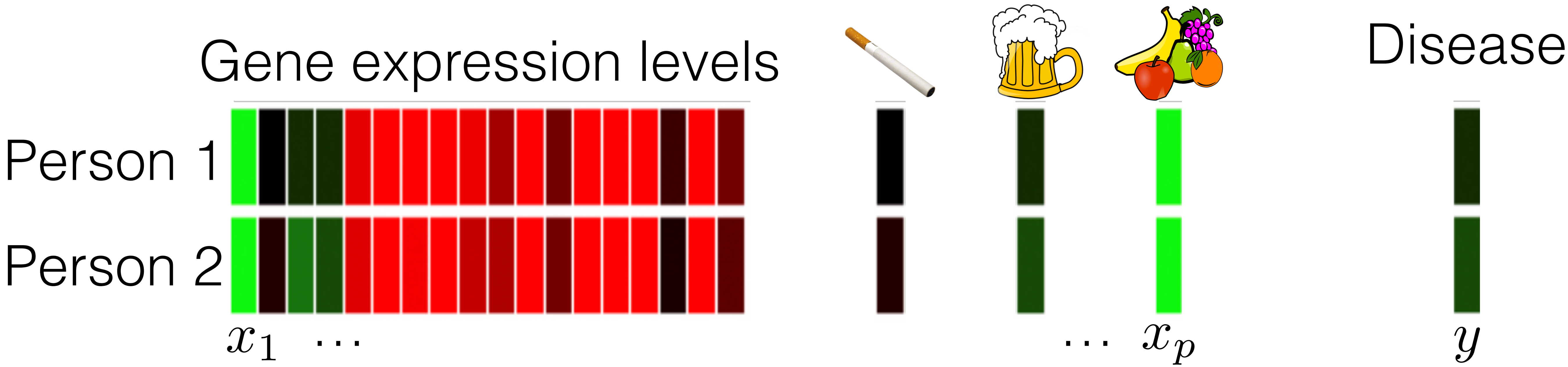

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- **Our solution**: using structure in covariates + sparsity assumptions to reduce to a problem *linear* in p

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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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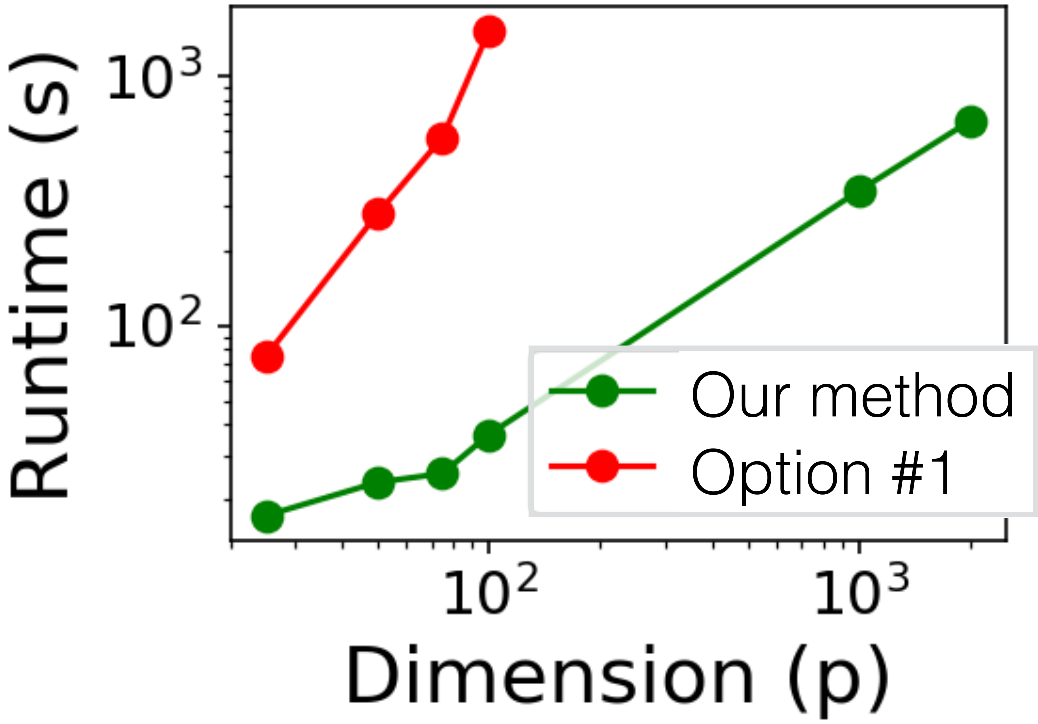

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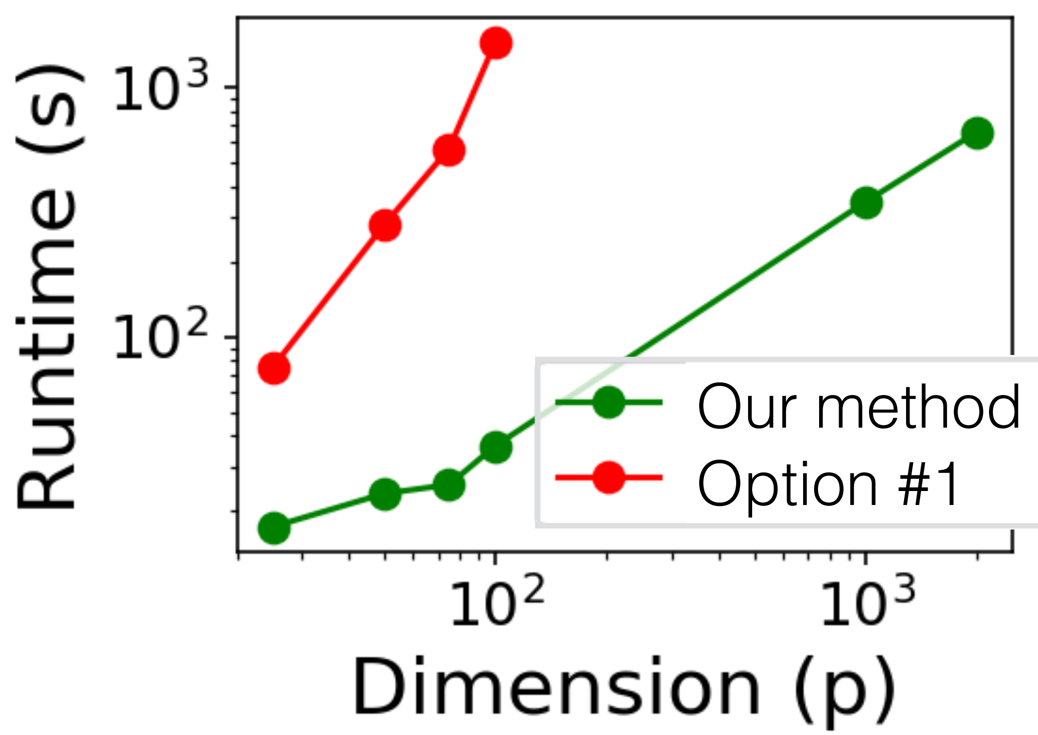

- Mixing (1000 iters Stan):
  - Option #1: all $\hat{R} > 1.05$
  - Our method: all $\hat{R} < 1.05$

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$$X^\top X$$

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

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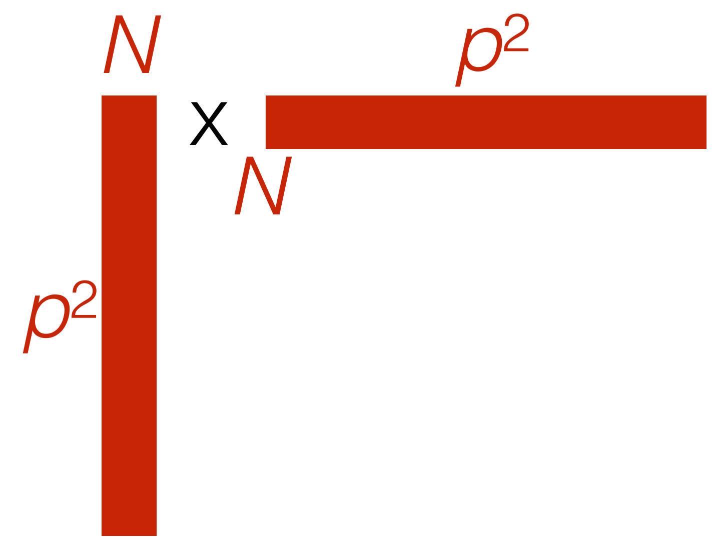

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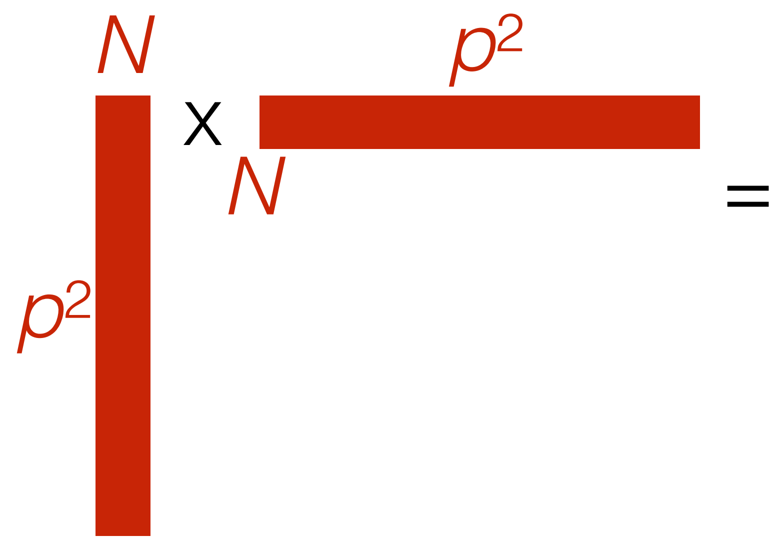

Kernel Interaction Sampler vs. Naive MCMC

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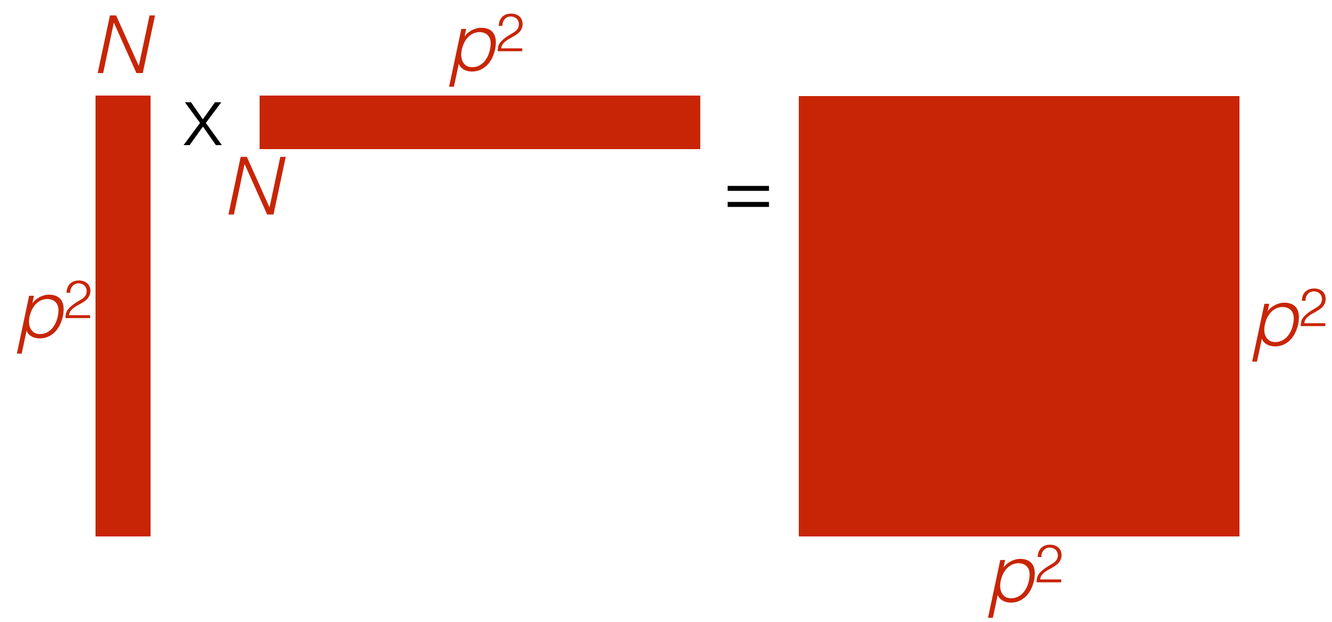

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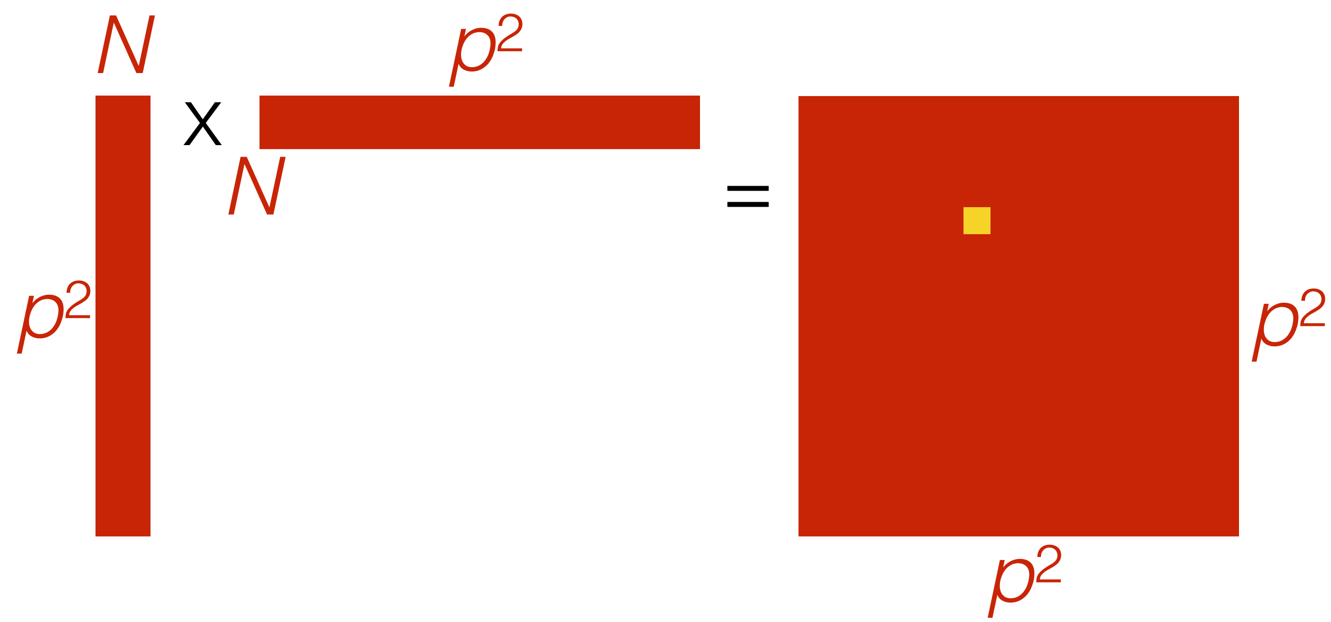

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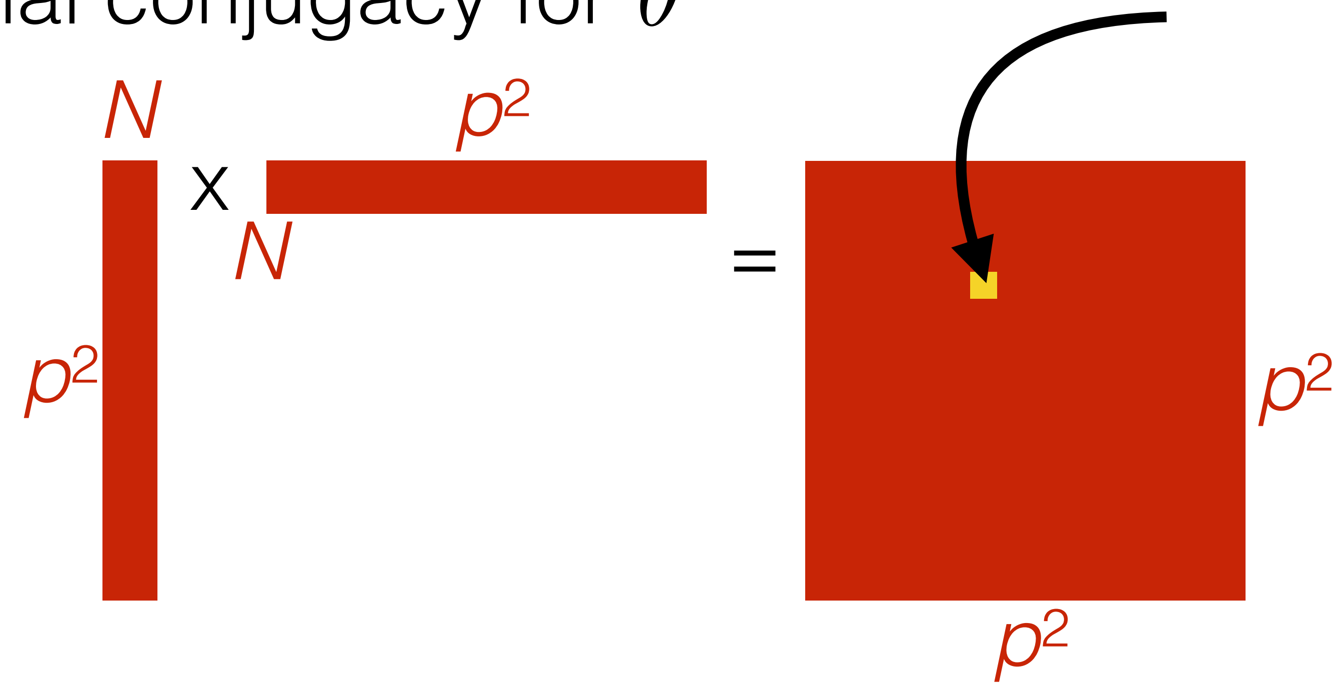

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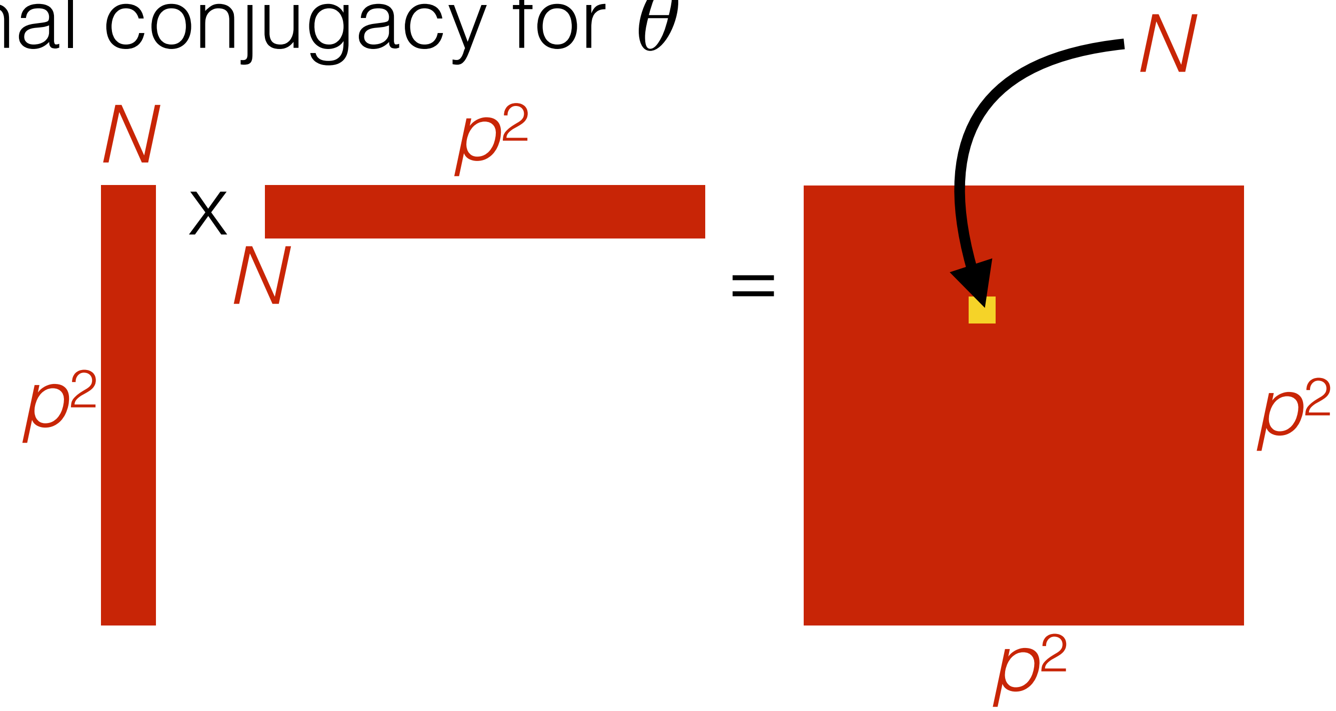

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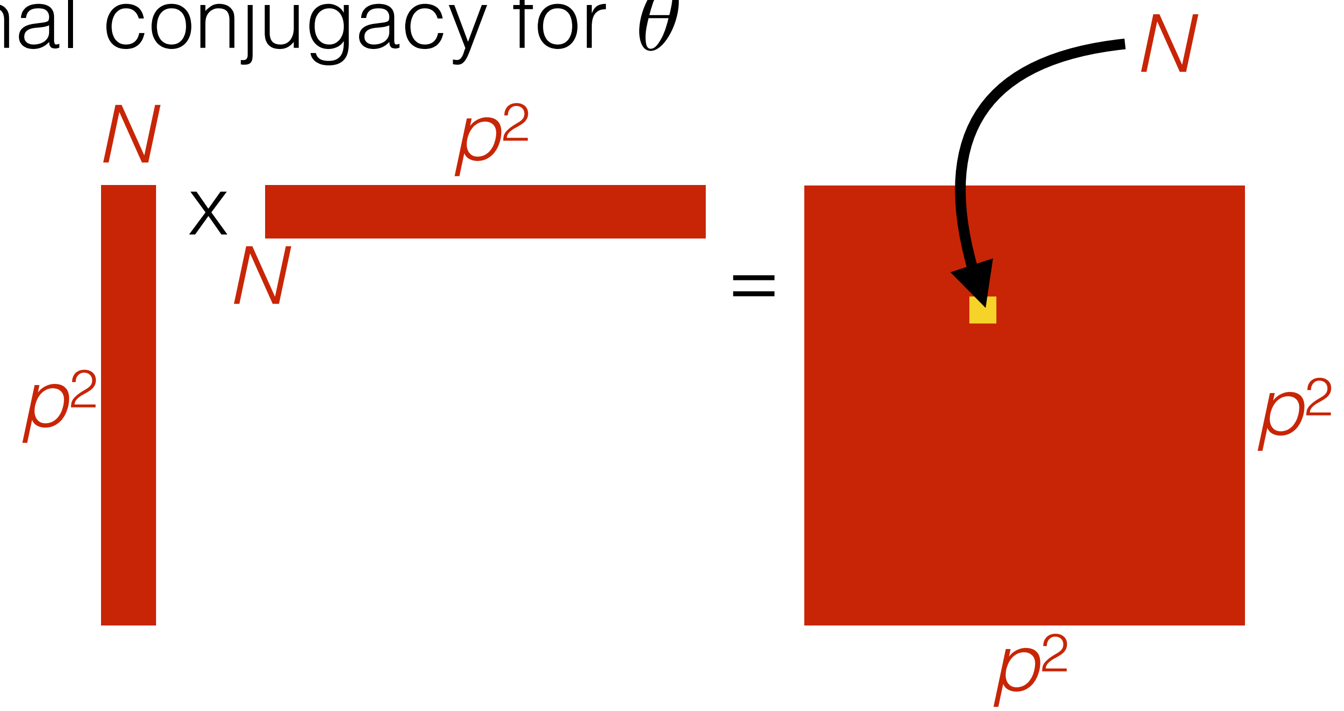

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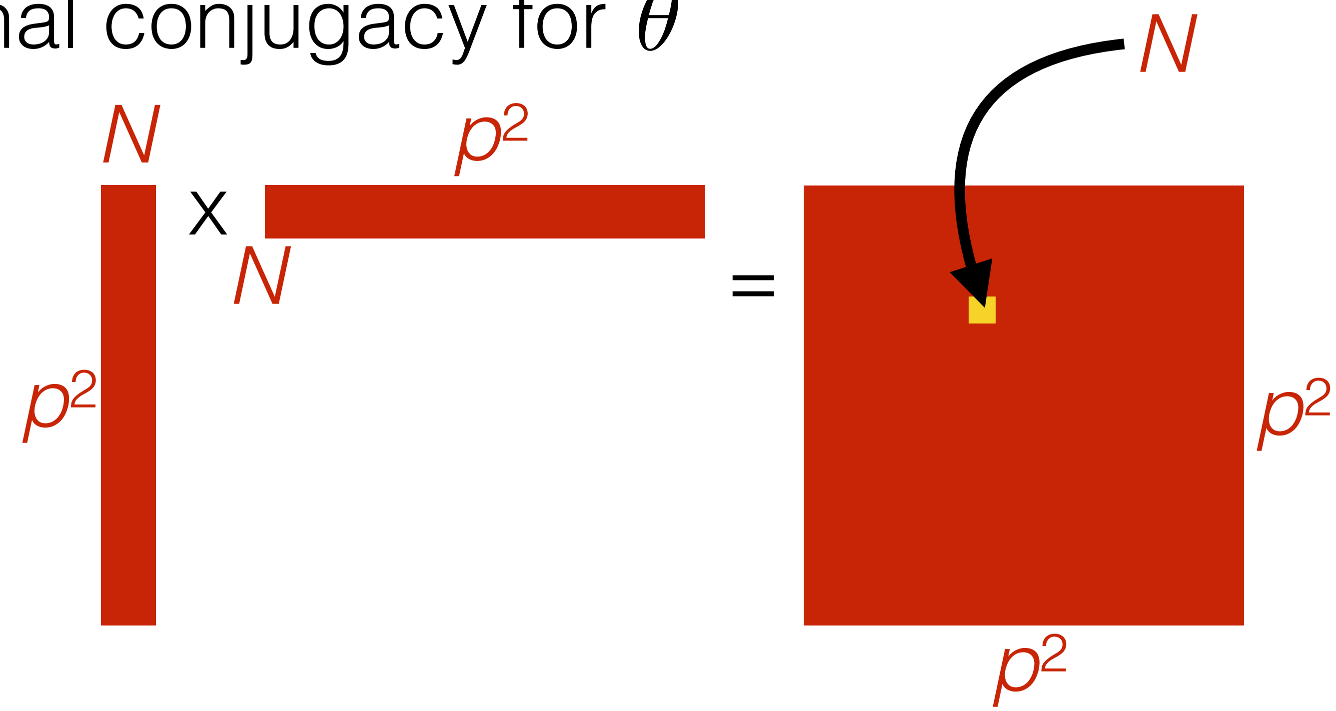

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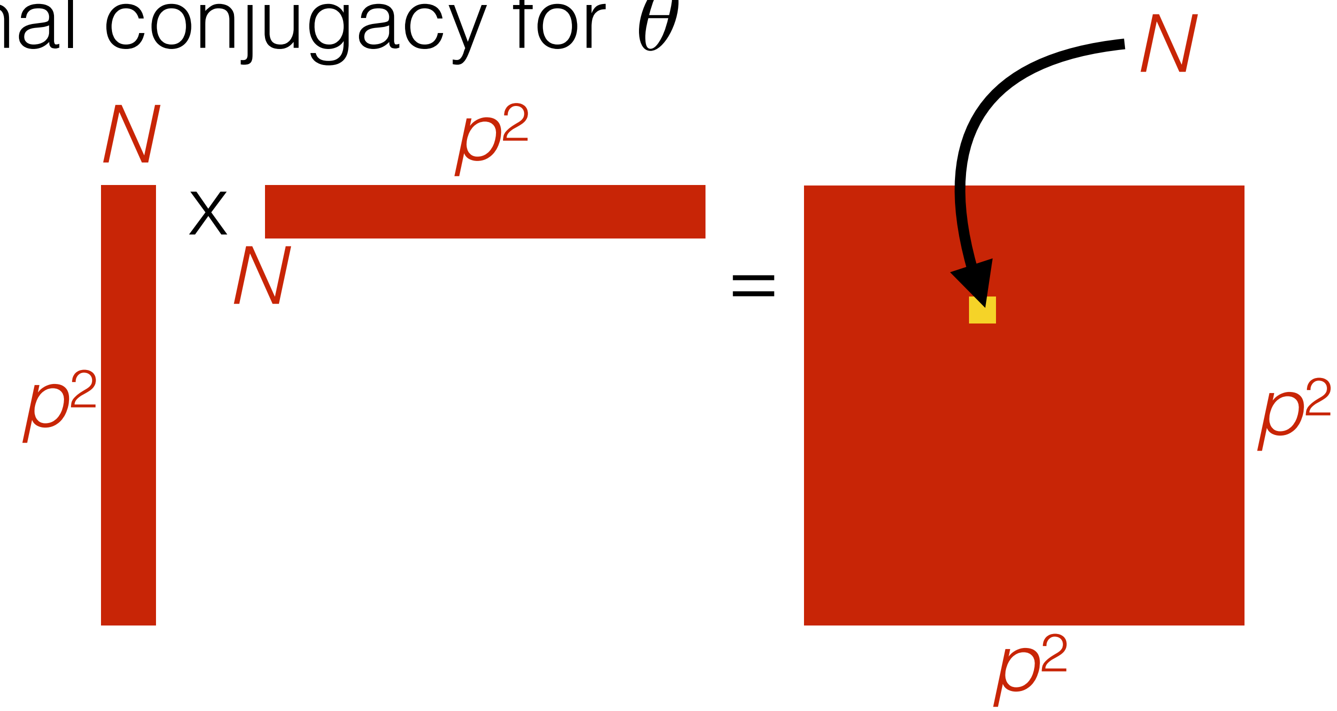

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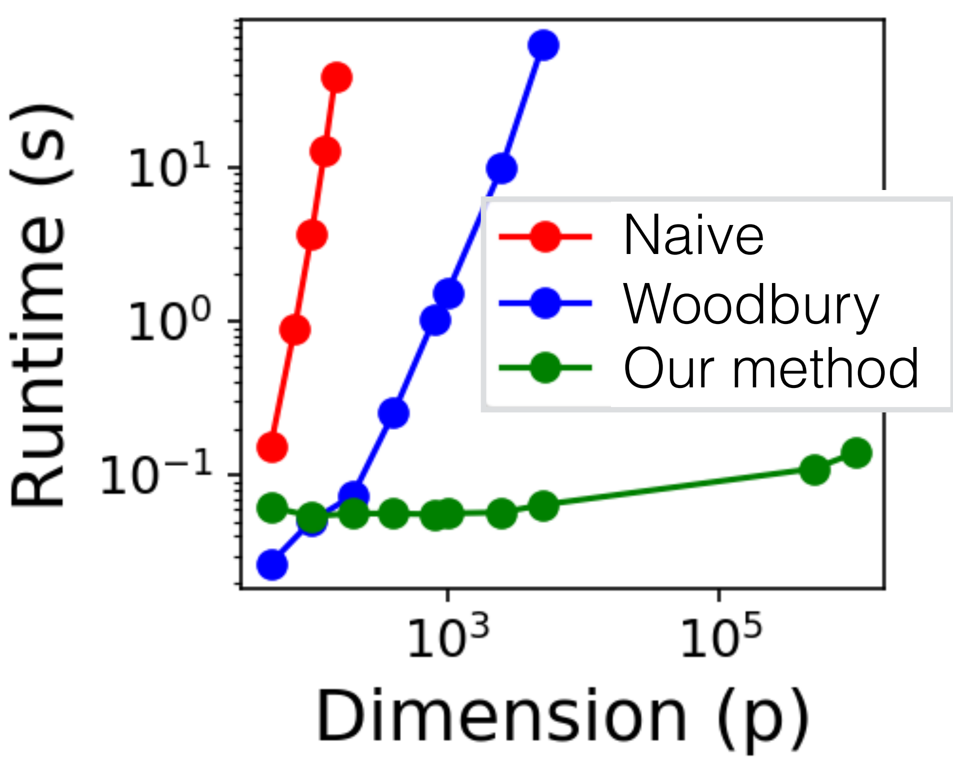

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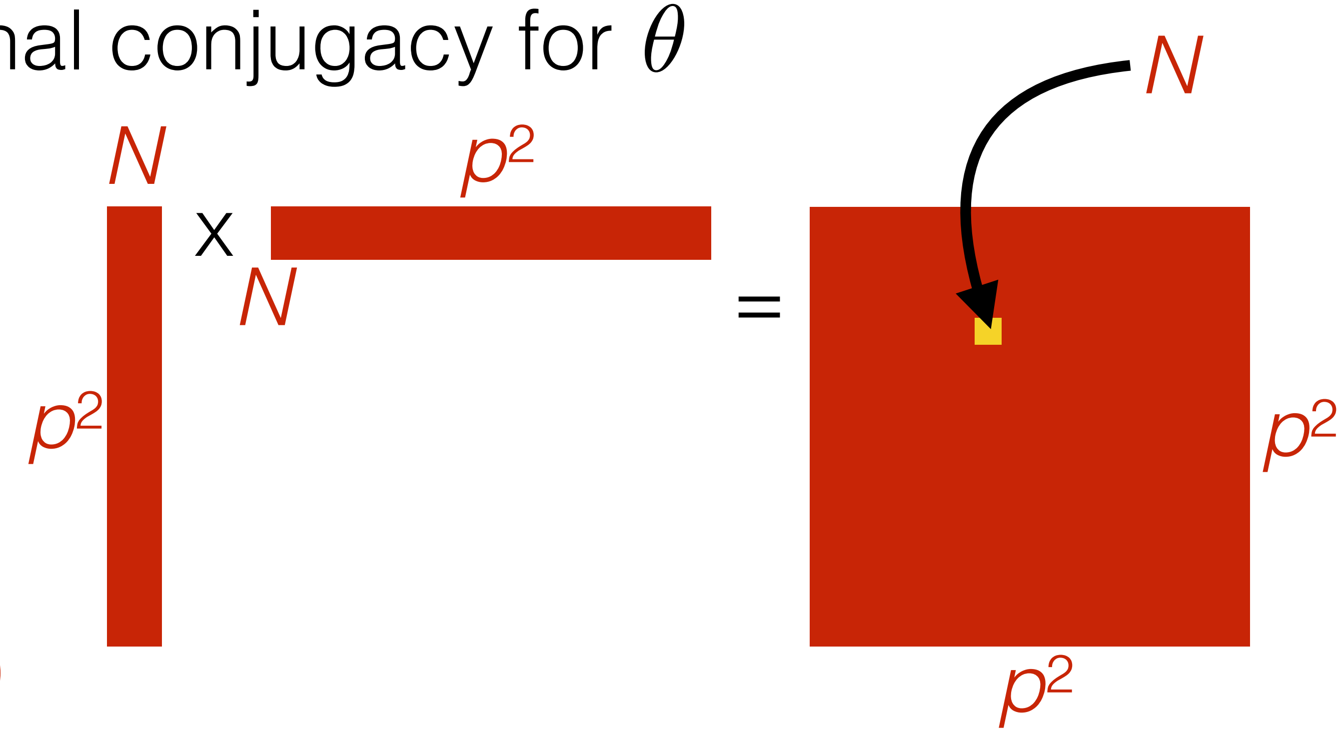

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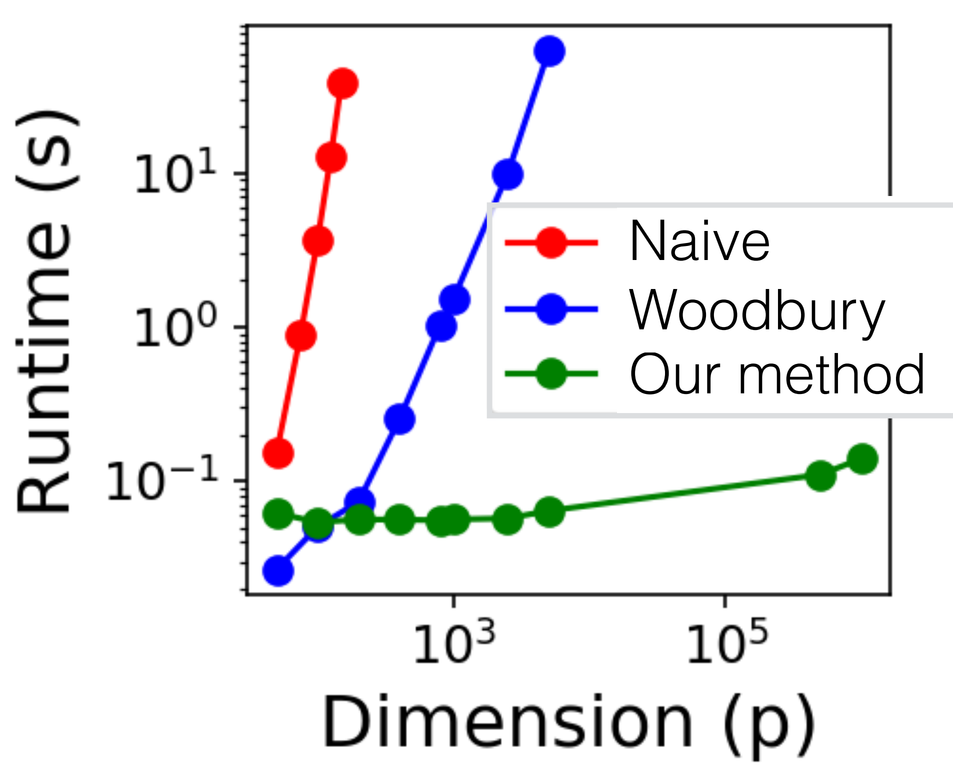

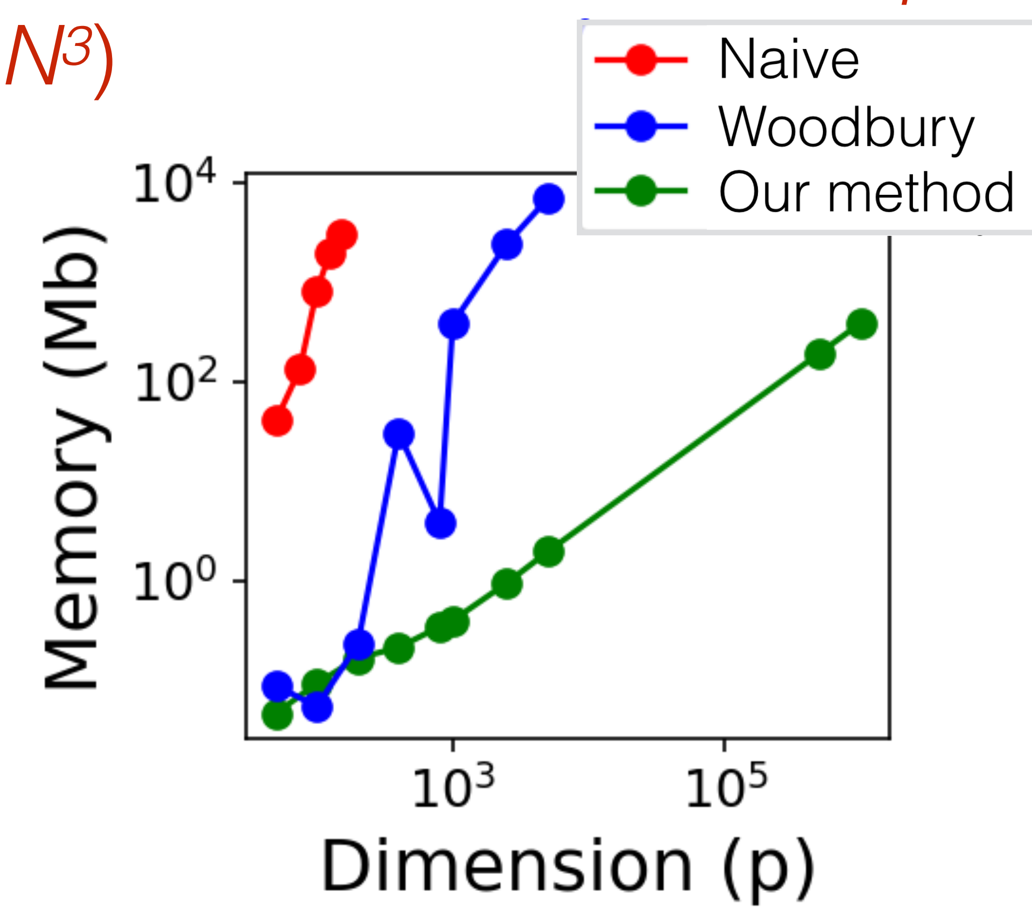

Kernel Interaction Sampler vs. Naive MCMC

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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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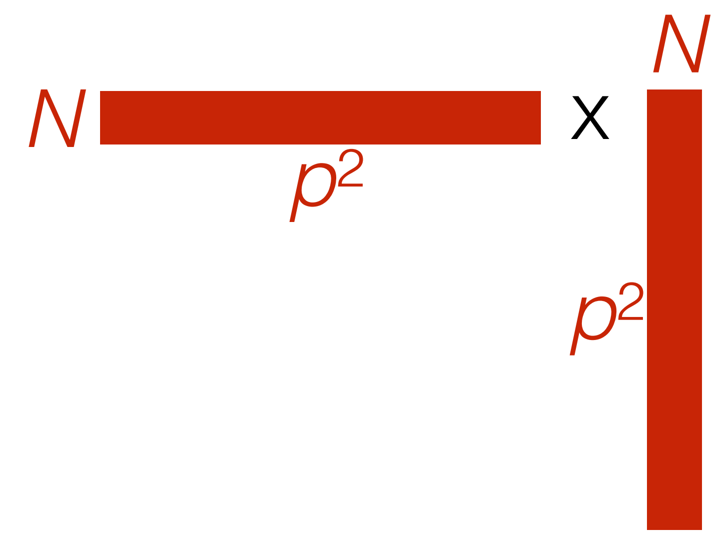

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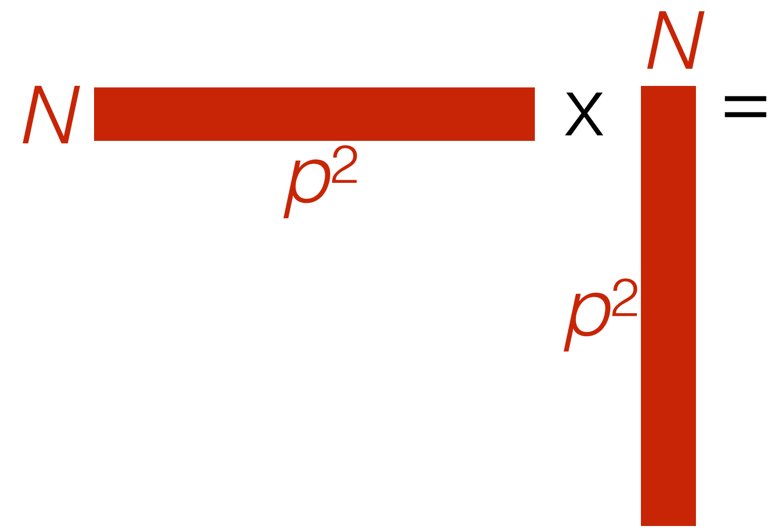

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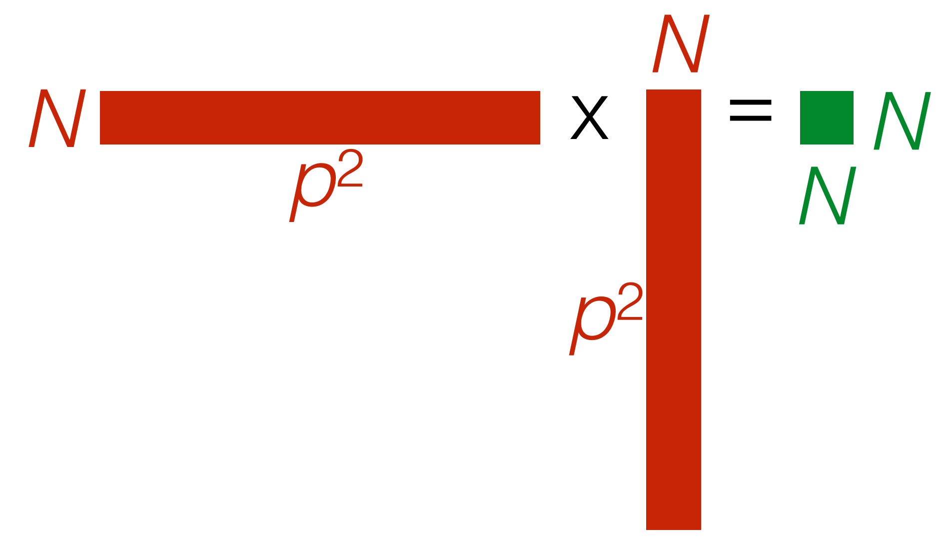

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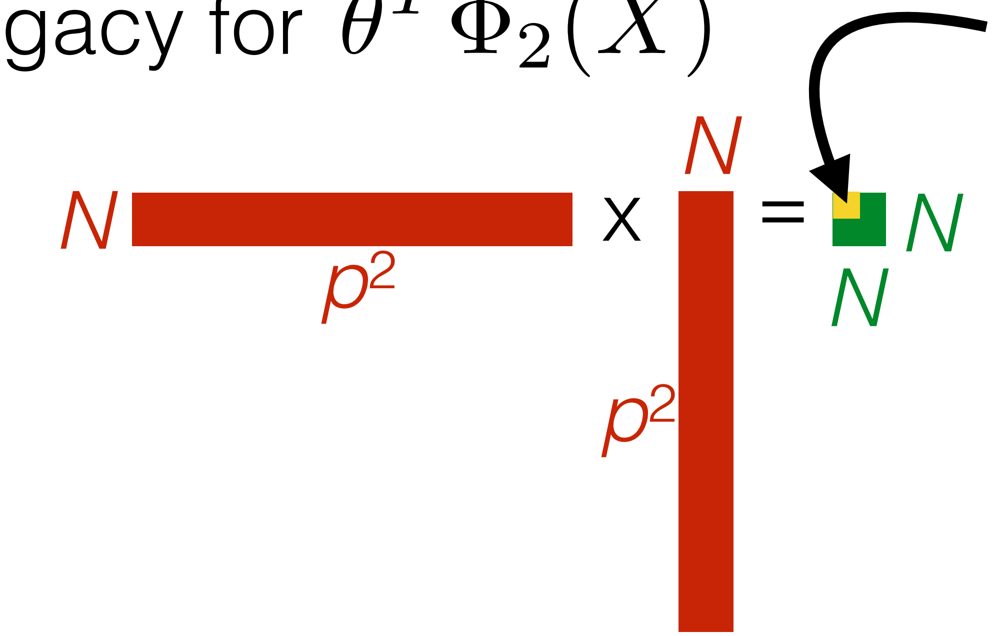

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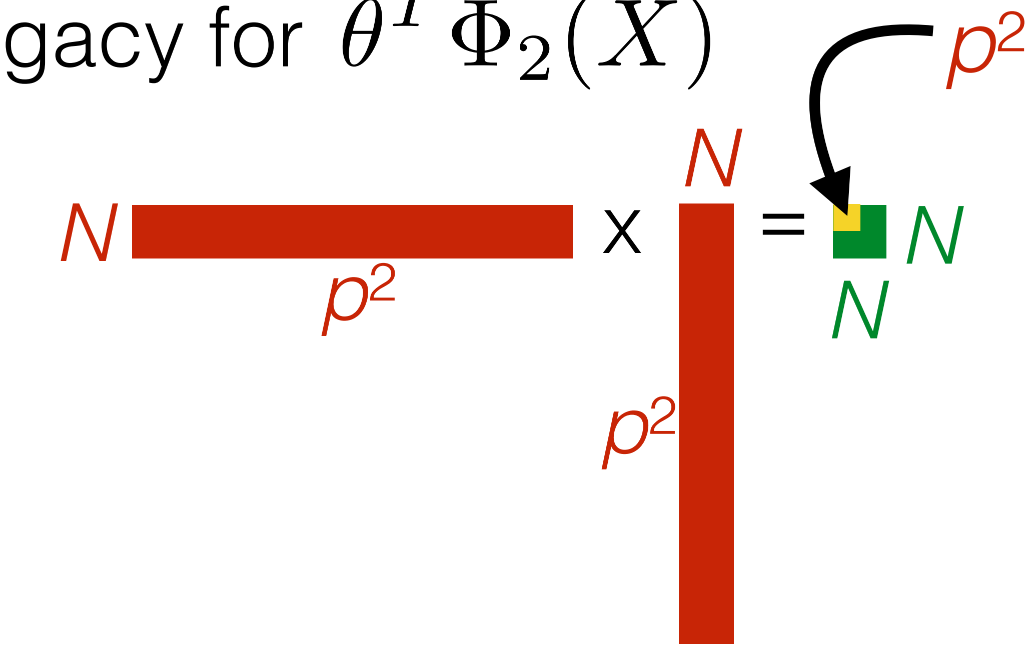

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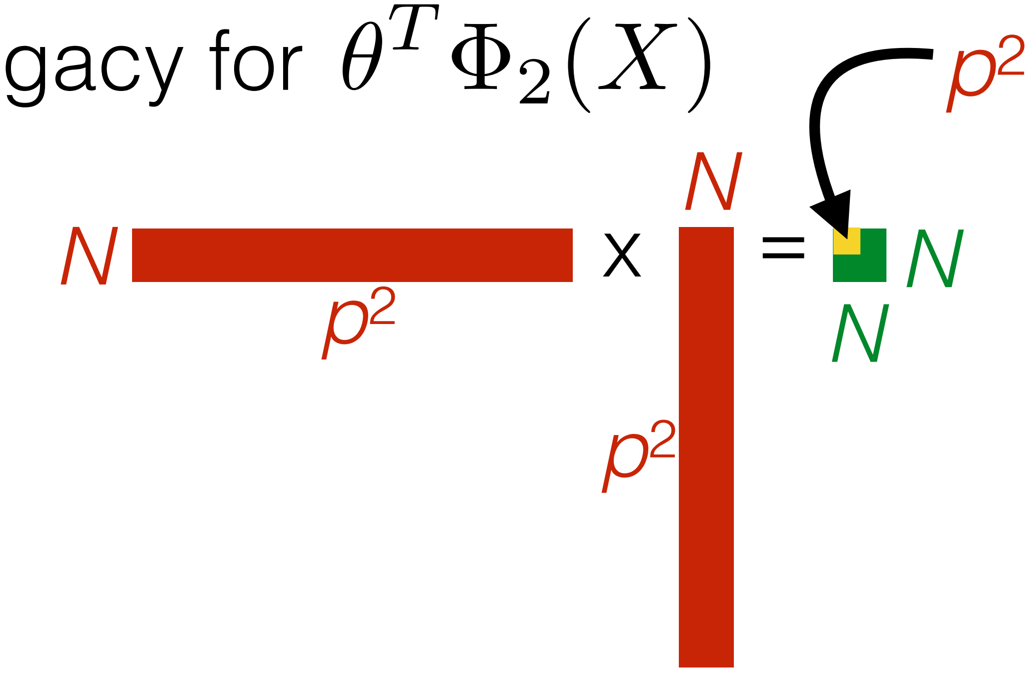

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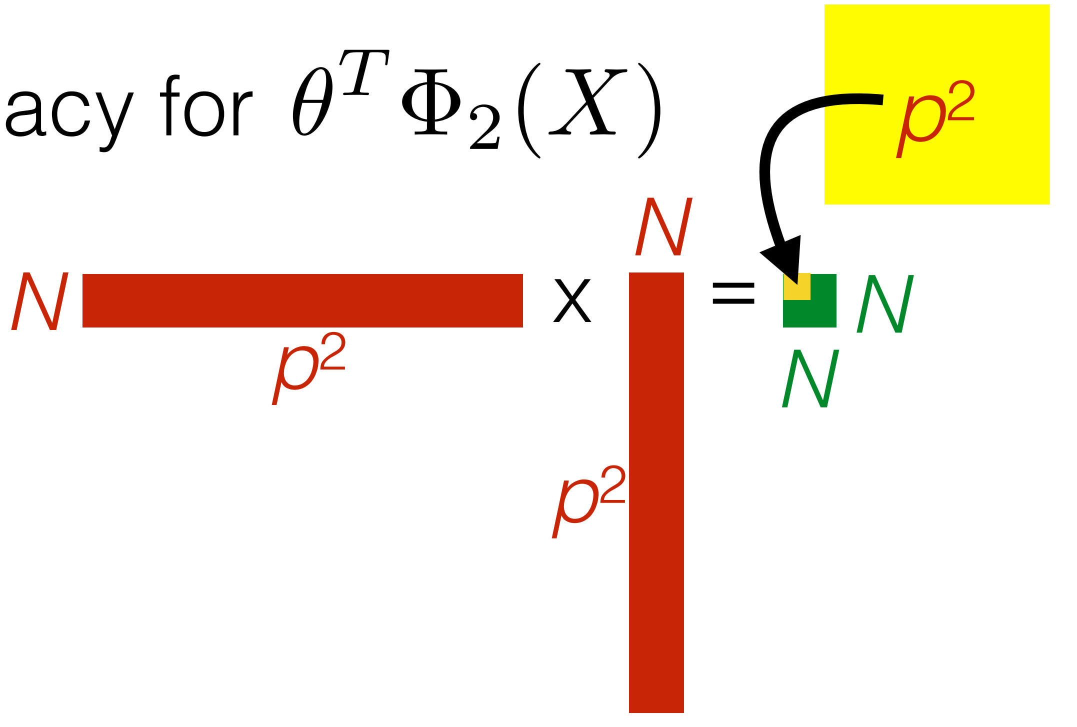

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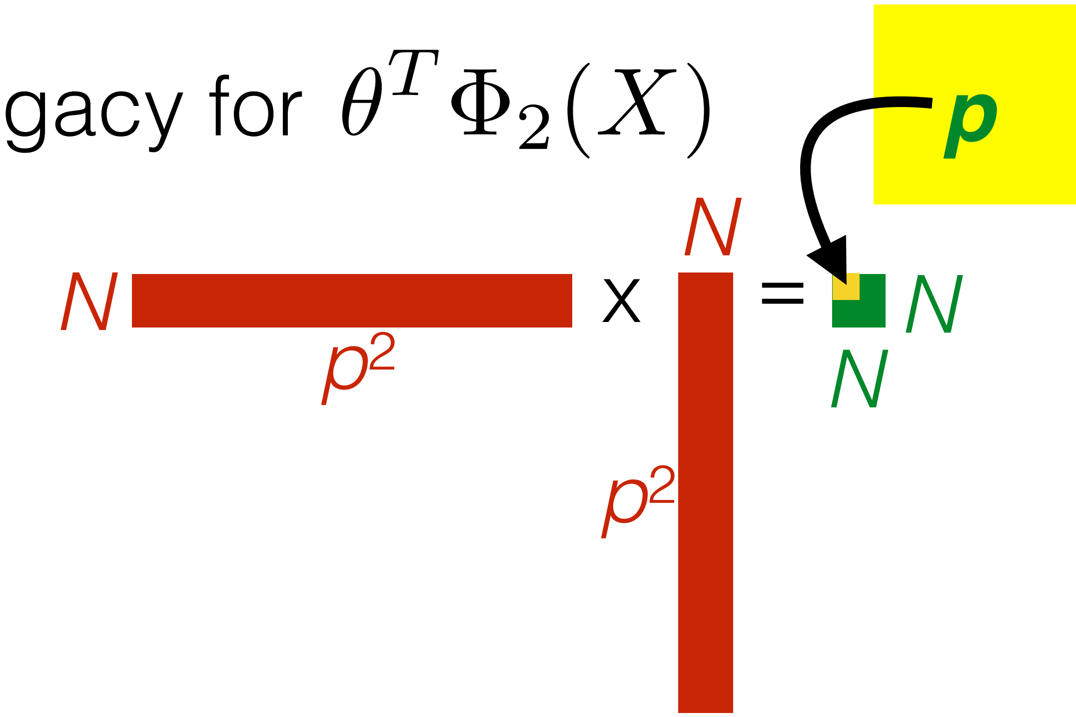

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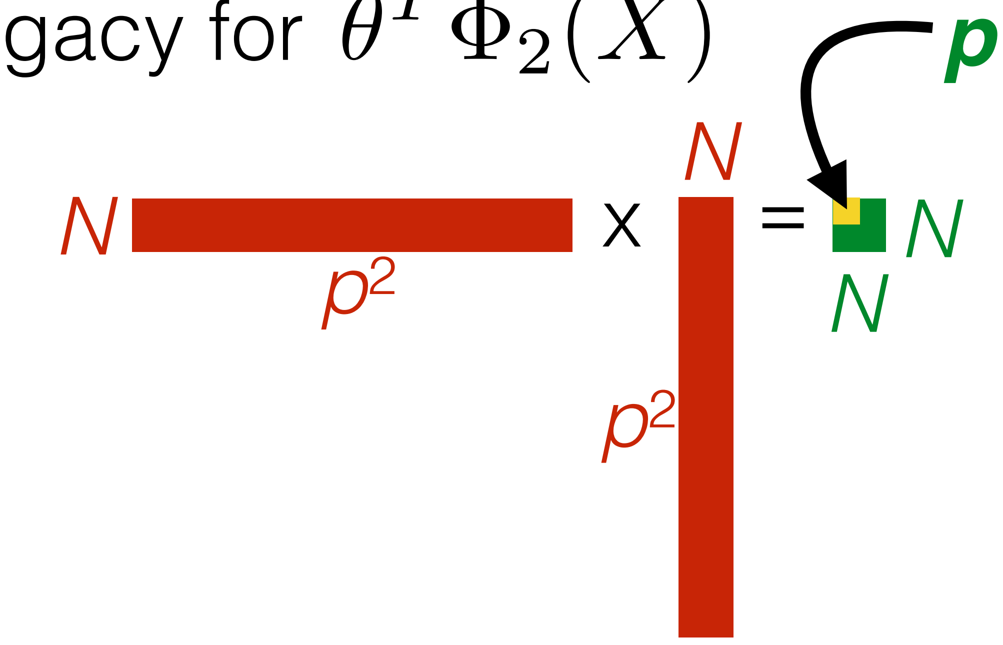

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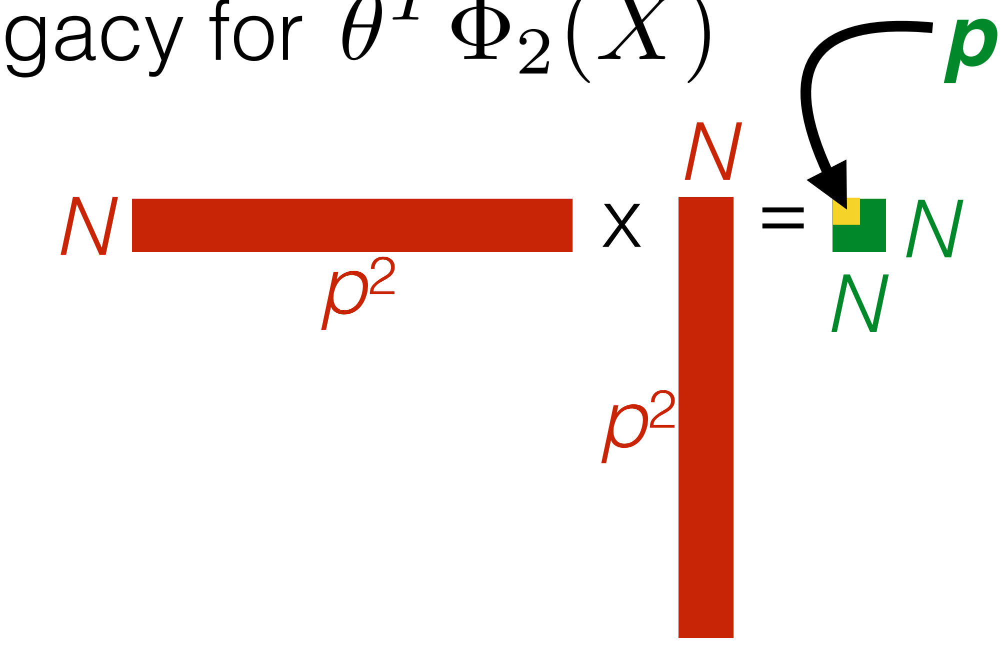

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- Step B: Find $k \ll p$ sparse main effects: takes $O(p)$ time
- Step C: Report just the k^2 strong-hierarchy interaction effects: takes $O(k^2)$ time

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- Setup: Discovering main and interaction effects
- Our method
  - A Bayesian generative model
  - Fast inference
  - Fast reporting of results
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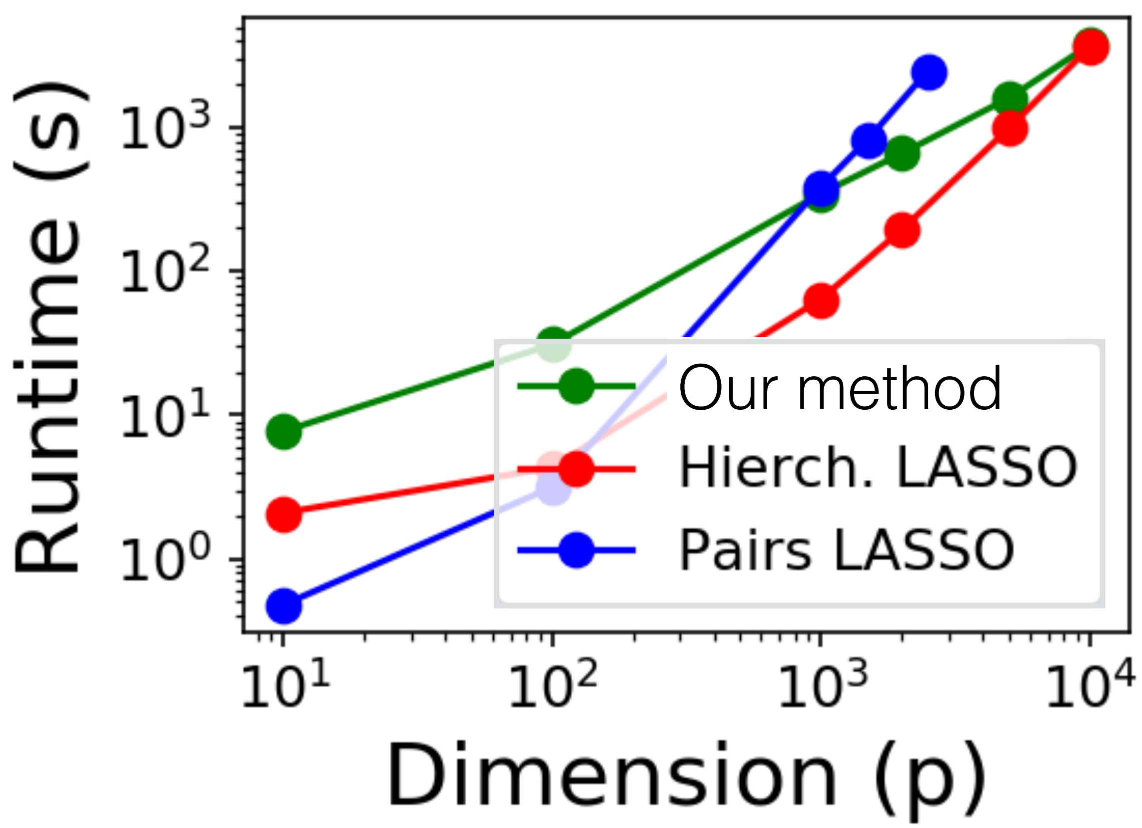

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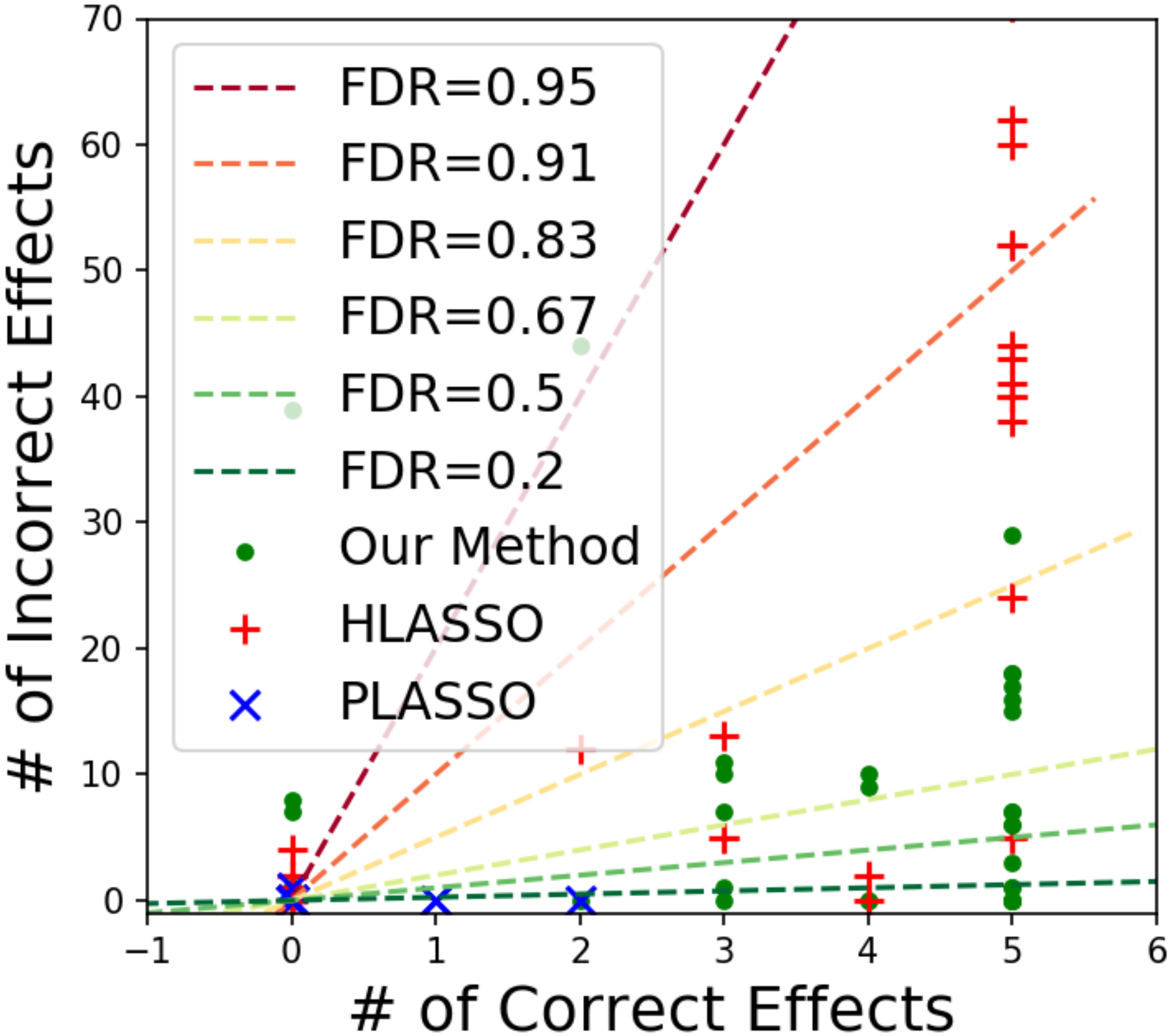
Main effects



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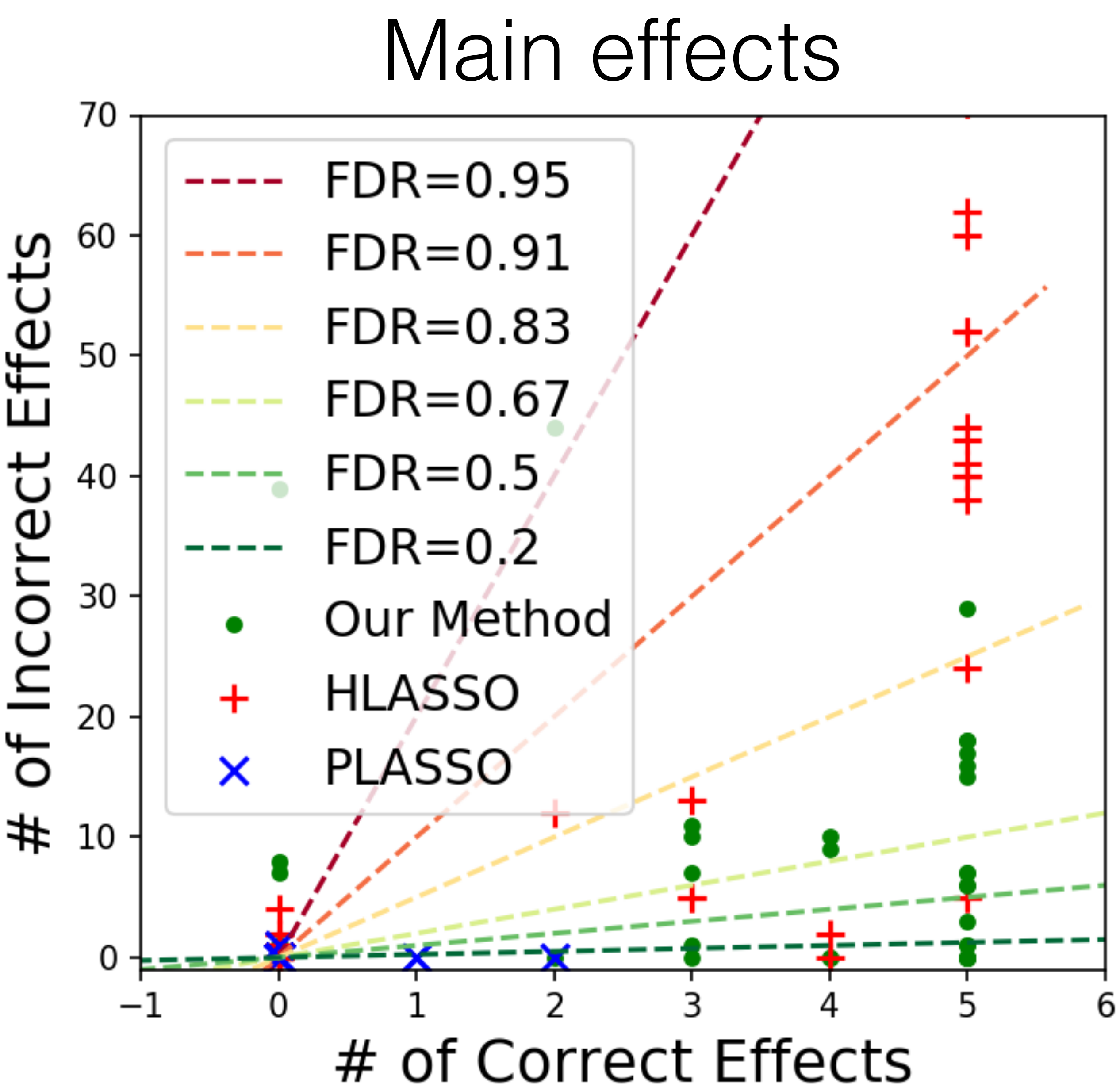

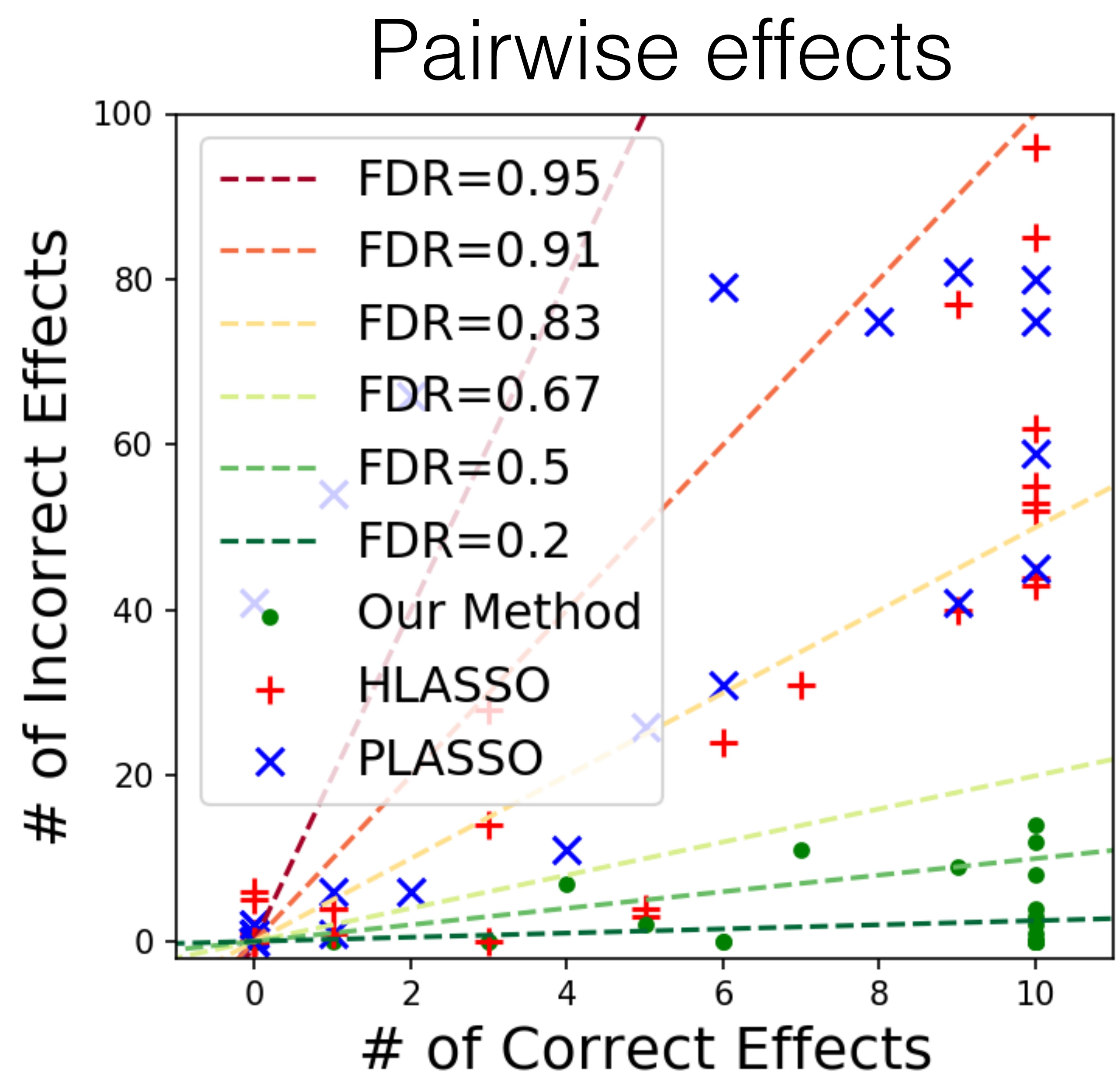

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METHOD	#MAIN	#PAIR
PLASSO	2 : 5	3 : 21

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METHOD	#MAIN	#PAIR
PLASSO	2 : 5	3 : 21
HLASSO	3 : 19	3 : 18

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Method	#Main	#Pair
Our method	**3 : 0**	**3 : 0**
PLASSO	**2 : 5**	**3 : 21**
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METHOD	#MAIN	#PAIR
PLASSO	4 : 0	2 : 78

Experiments: Real data

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

Experiments: Real data

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METHOD	#MAIN	#PAIR
Our method	**3 : 0**	**1 : 0**
PLASSO	**4 : 0**	**2 : 78**
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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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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

Thanks to Pyro contributors! Martin Jankowiak, Du Phan, Neeraj Pradhan

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

Conclusions

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

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- Improve scaling in *N*

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Conclusions

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

Up next:

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- Improve scaling in N
- Genetics (epistasis) application, etc

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Sparse Kernel Interaction Model (SKIM)

Likelihood

$$y^{(n)} \sim \mathcal{N}(\theta^\top \Phi_2(x^{(n)}), \sigma^2)$$

s.t. $\Phi_2^\top(x) := [1, x_1, \ldots, x_p, x_1^2, x_1 x_2, \ldots, x_p^2]$

SKIM prior

$$\sigma^2 \sim p(\sigma^2)$$

$$\theta_{x_i} \sim \mathcal{N}(0, m^2 \tilde{\kappa}_i^2)$$ ➔ sparsity

$$\theta_{x_i x_j} \sim \mathcal{N}(0, \xi^2 \tilde{\kappa}_i^2 \tilde{\kappa}_j^2)$$ ➔ strong hierarchy

$$\theta_{x_i^2} \sim \mathcal{N}(0, \psi^2 (\tilde{\kappa}_i^2)^2)$$

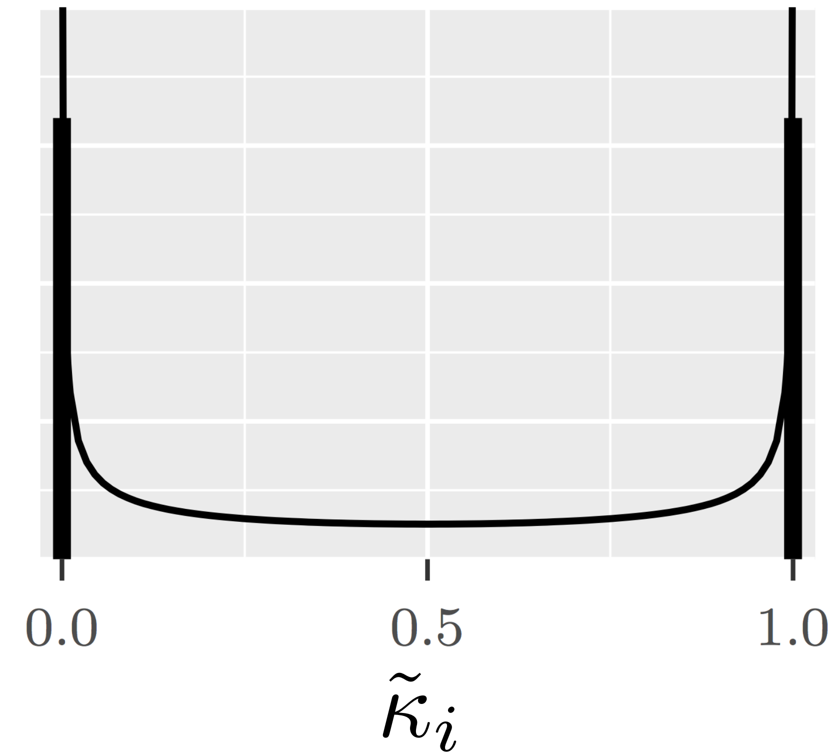
(Compare to Chipman 1996, Griffin & Brown 2017)

$$\theta_0 \sim \mathcal{N}(0, c^2)$$

$\tilde{\kappa}_i$: regularized horseshoe priors [Carvalho et al 2009; Piironen, Vehtari 2017]

m^2, ξ^2, ψ^2, c^2 : inverse gamma priors

[Piironen, Vehtari 2017]



- **Challenge**: p^2 parameters
- **Helpful**: Conditional conjugacy / Gaussian process
- **Note**: Specific case of a broader class of models

Experiments: Simulated, Estimation

- 36 different simulated data sets (so know true effects)
  - Up to p = 500 ➔ ≈125,000 total parameters