

Fast Discovery of Pairwise Interactions in High Dimensions using Bayes

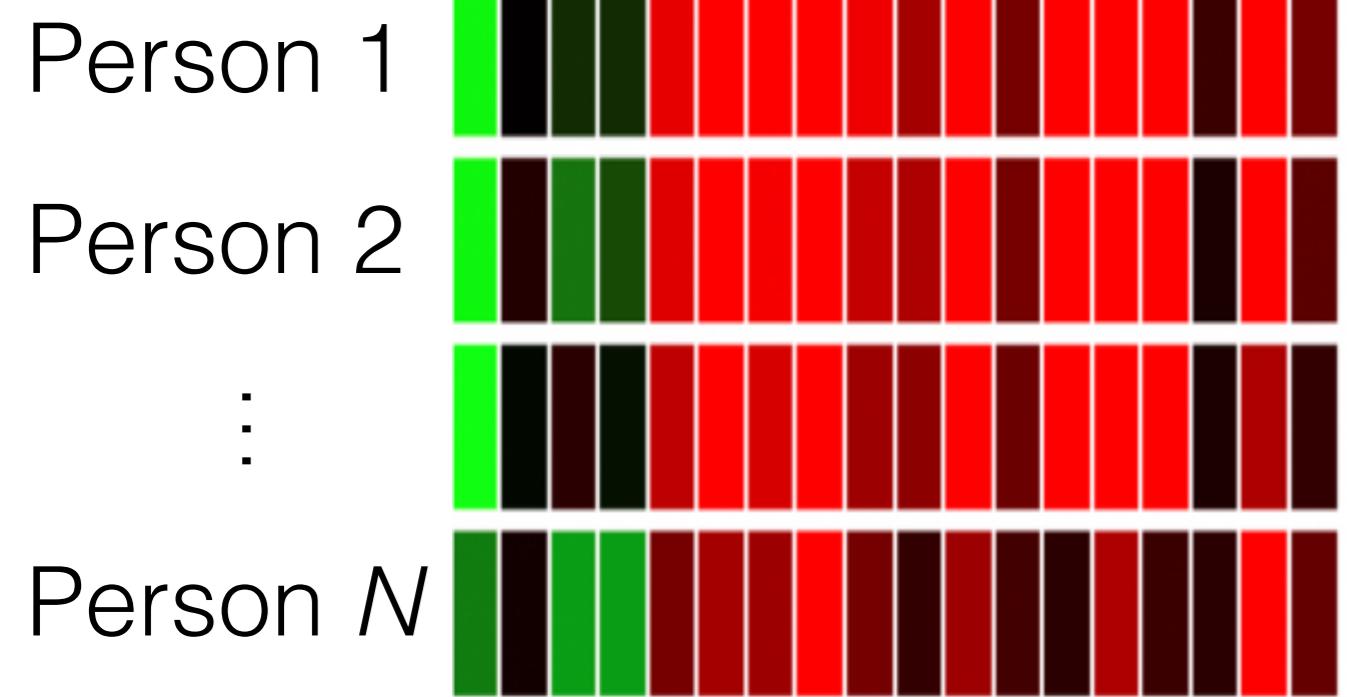
Tamara Broderick

Associate Professor
EECS, MIT

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



Gene expression levels



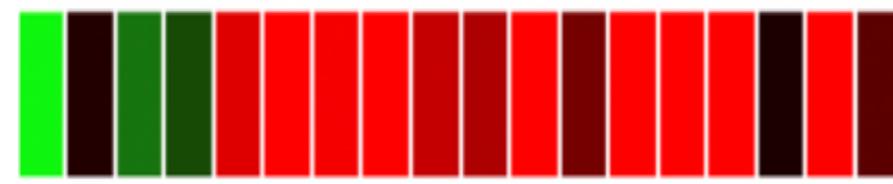
Environmental factors

Gene expression levels

Person 1

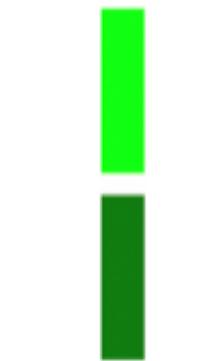
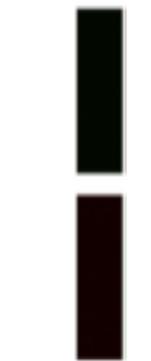
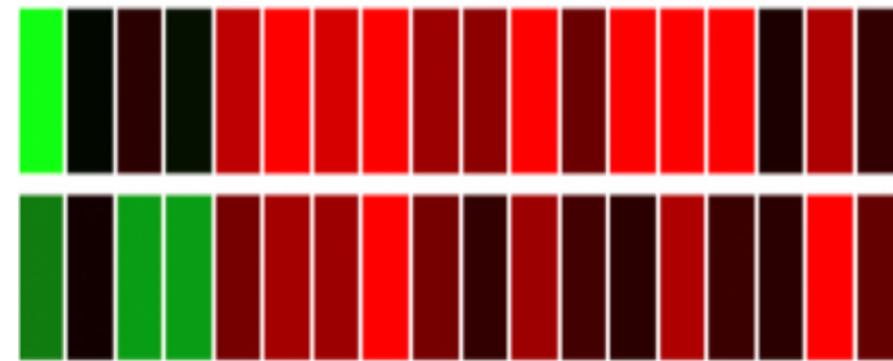


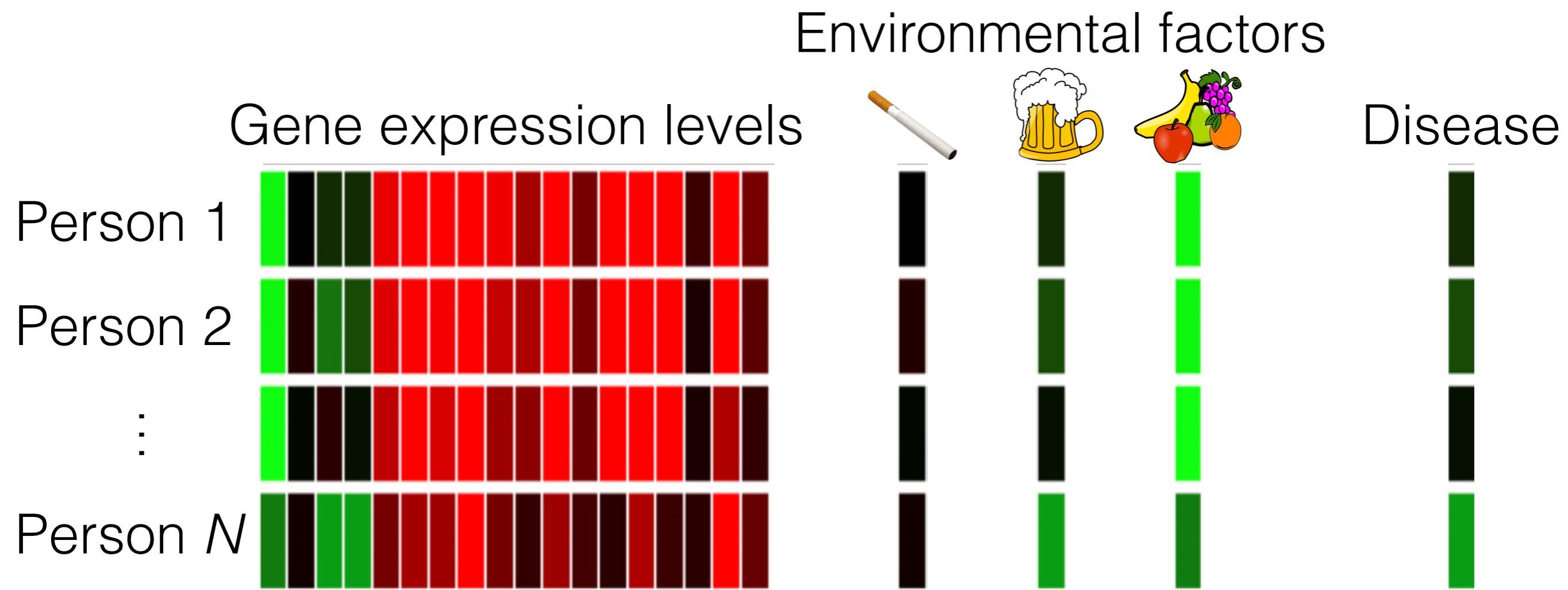
Person 2



:

Person N





Environmental factors



Gene expression levels

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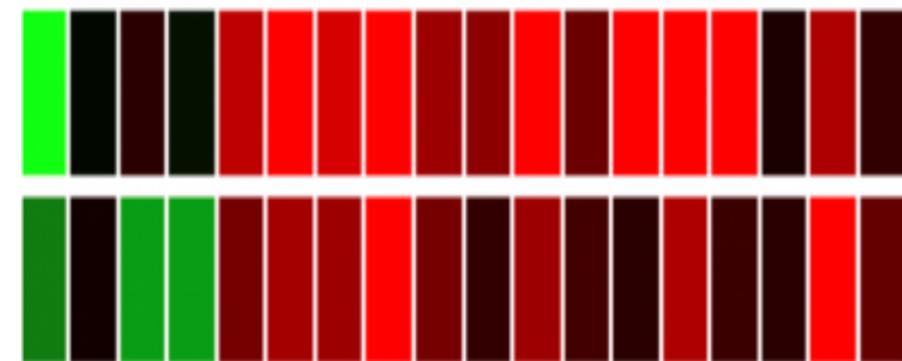


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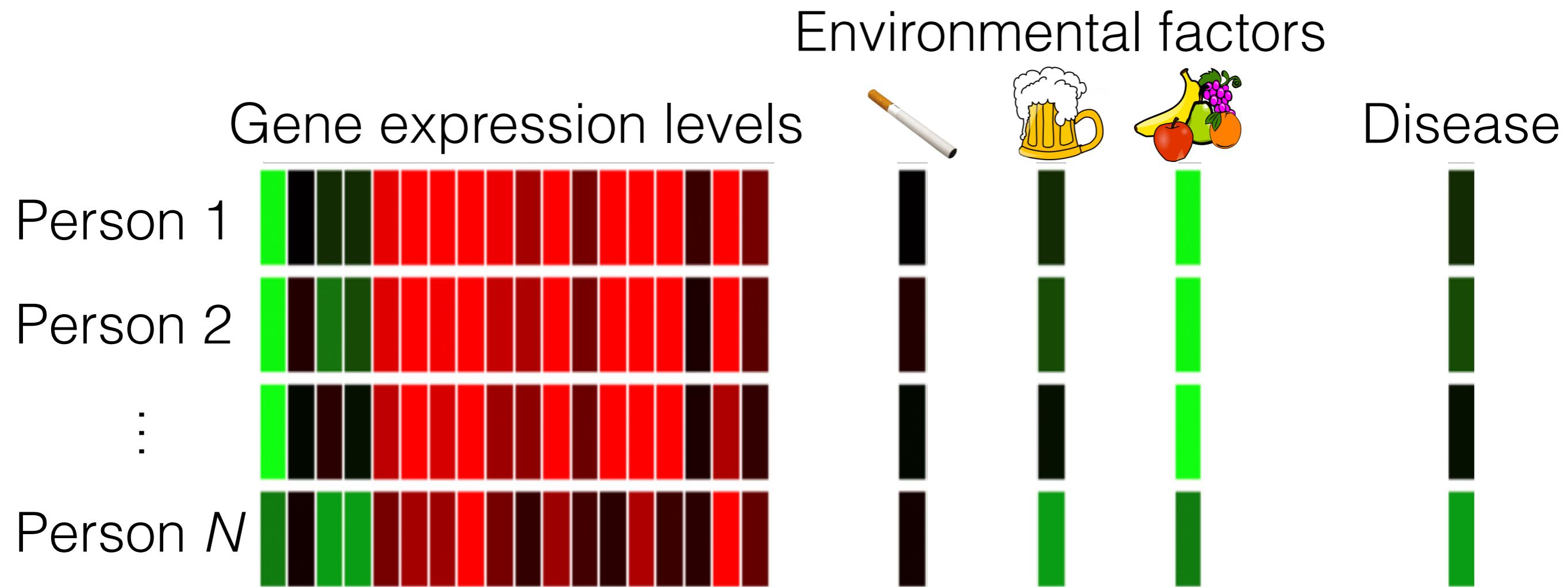
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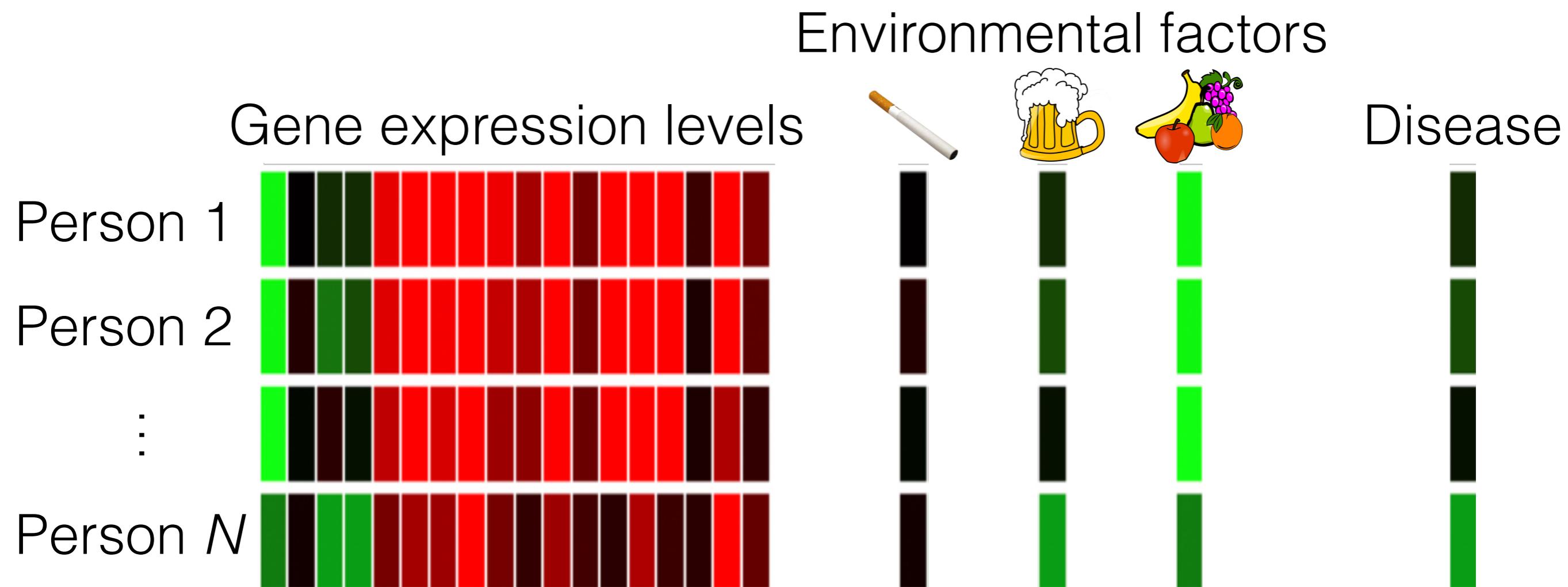
Disease



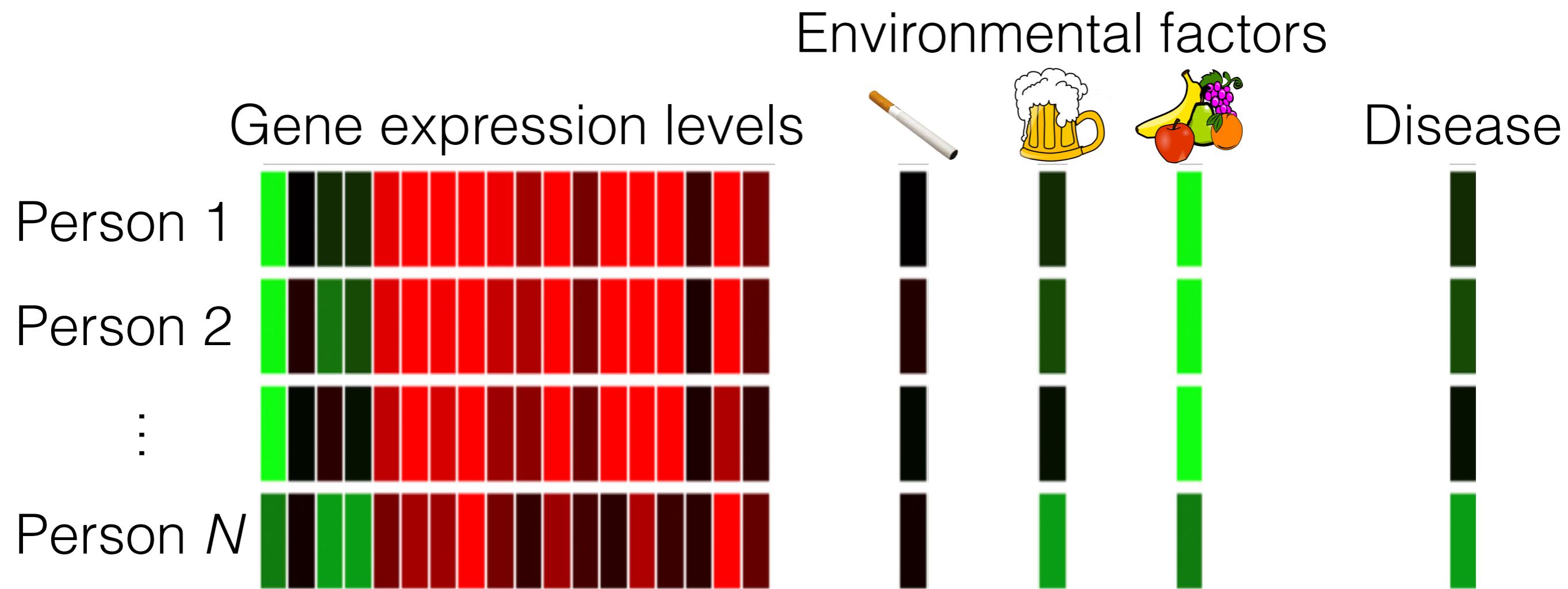
- Which genes/factors are associated with a disease?



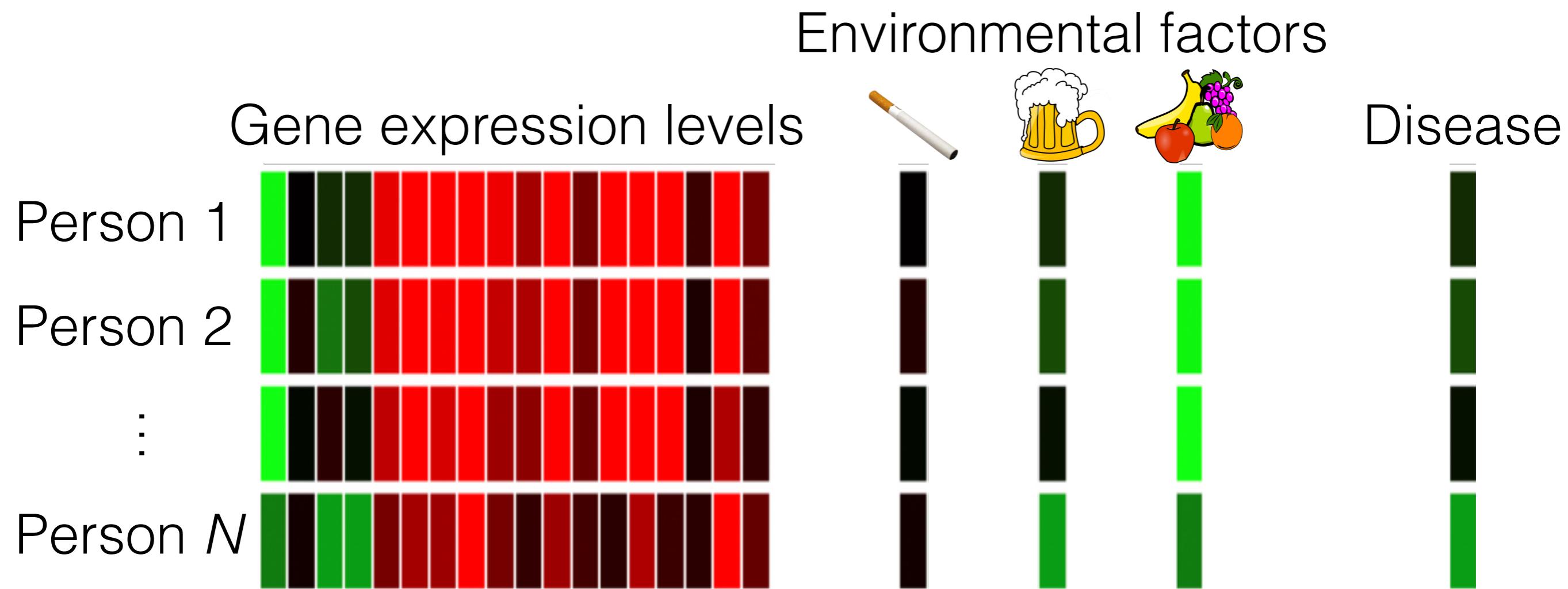
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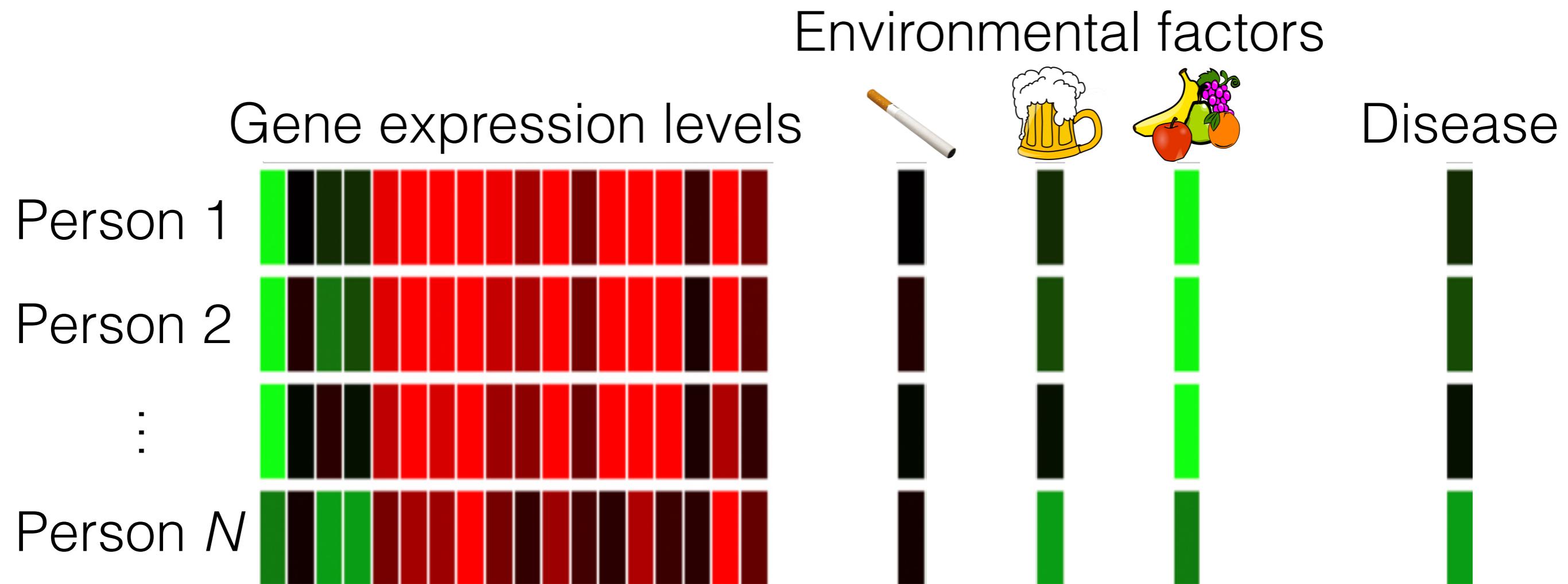


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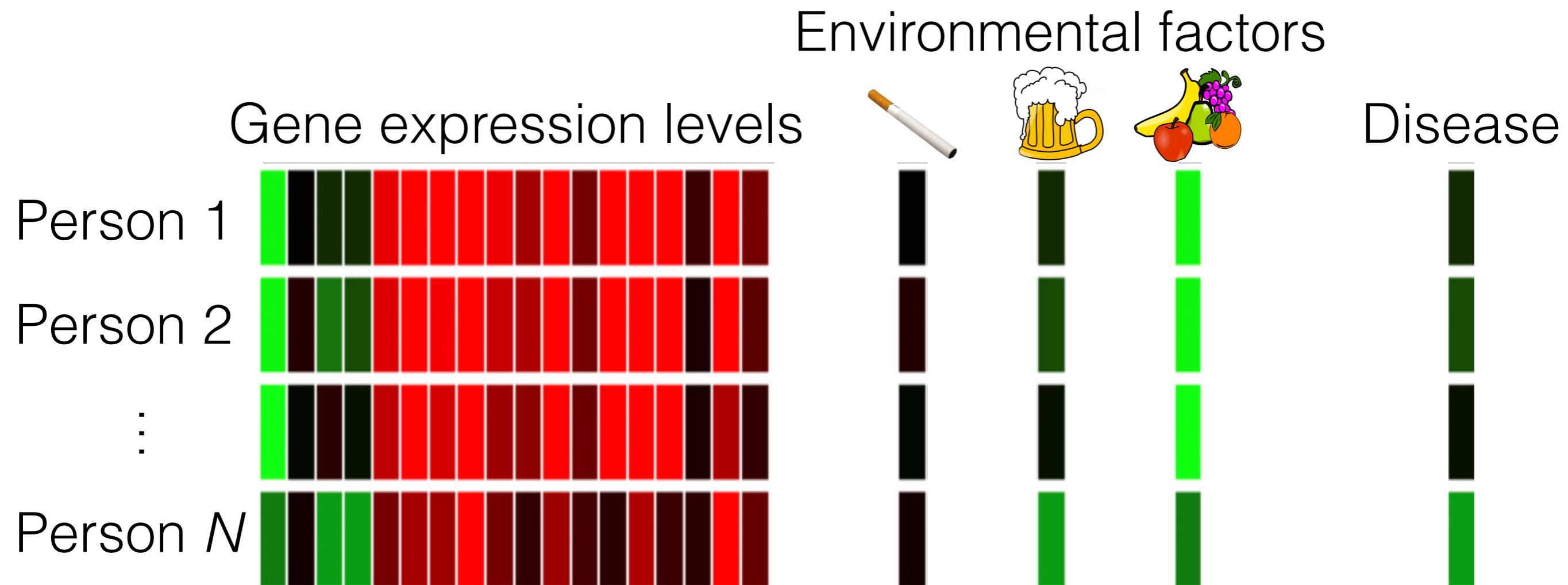
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Pairwise interactions in high dimensions



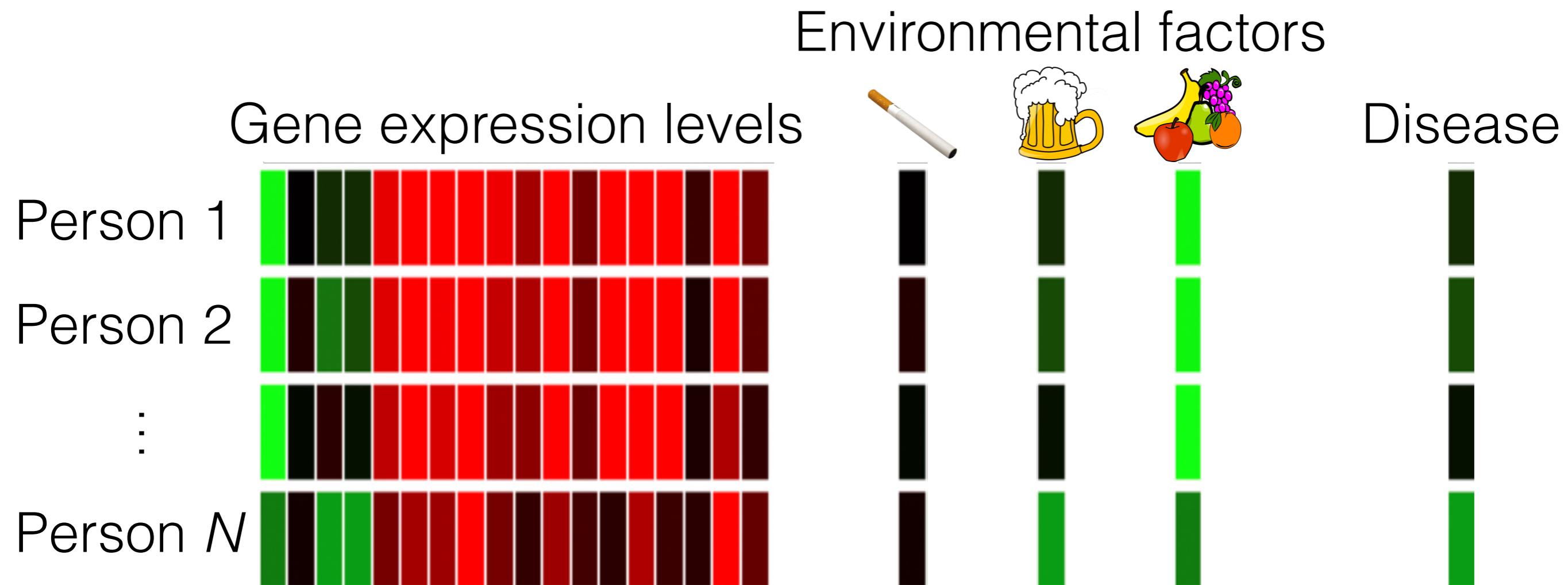
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- **We provide:** Fast, accurate (Bayes) method for interaction discovery
 - Better scaling in p & better accuracy than LASSO-based methods.
Orders of magnitude faster than naive Bayesian inference

Roadmap

Roadmap

- Setup: Discovering main and interaction effects

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- Our method

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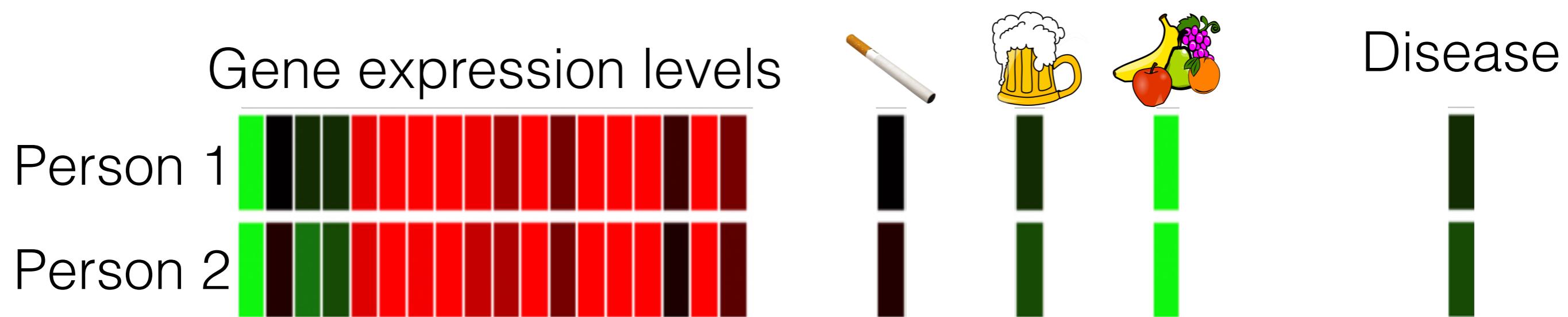
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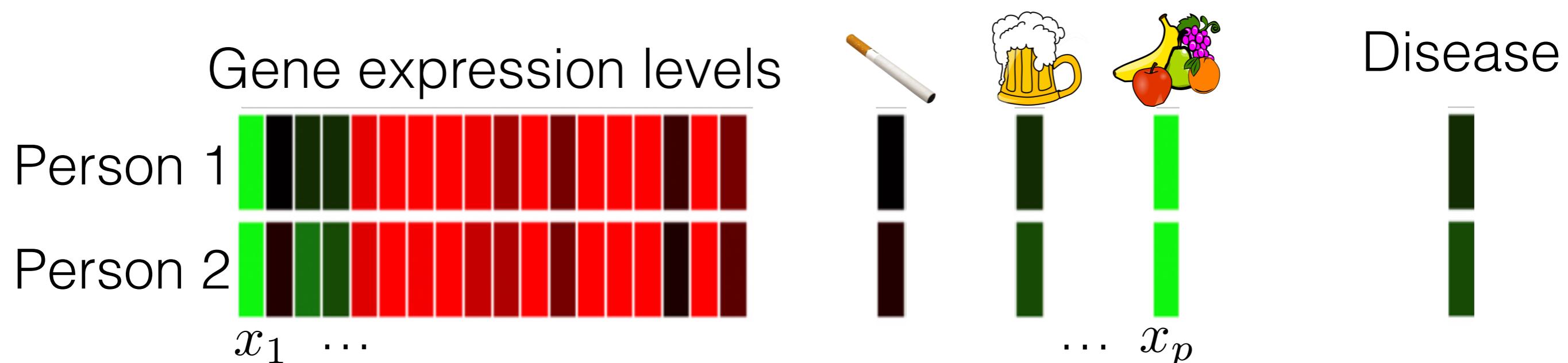
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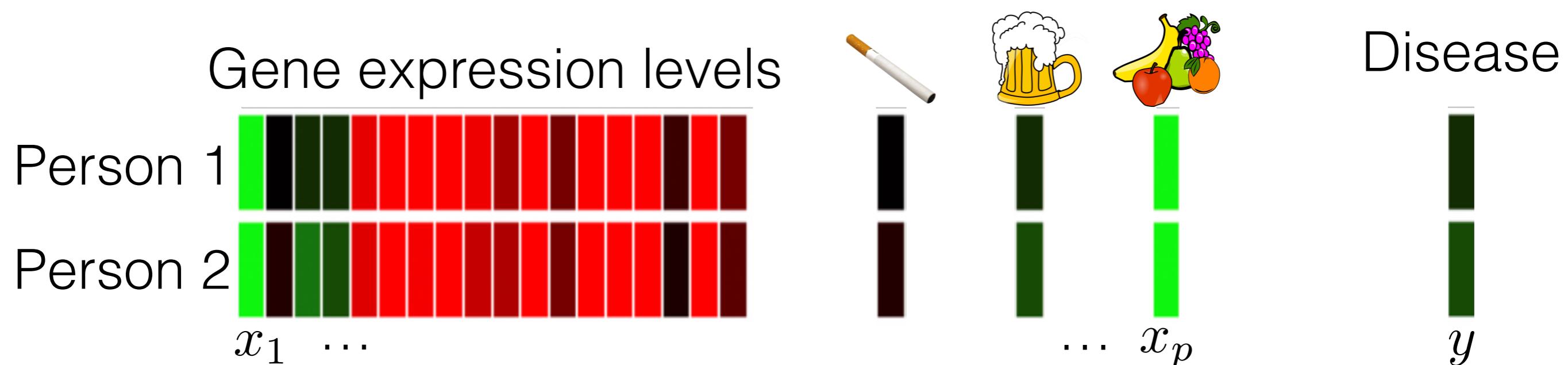
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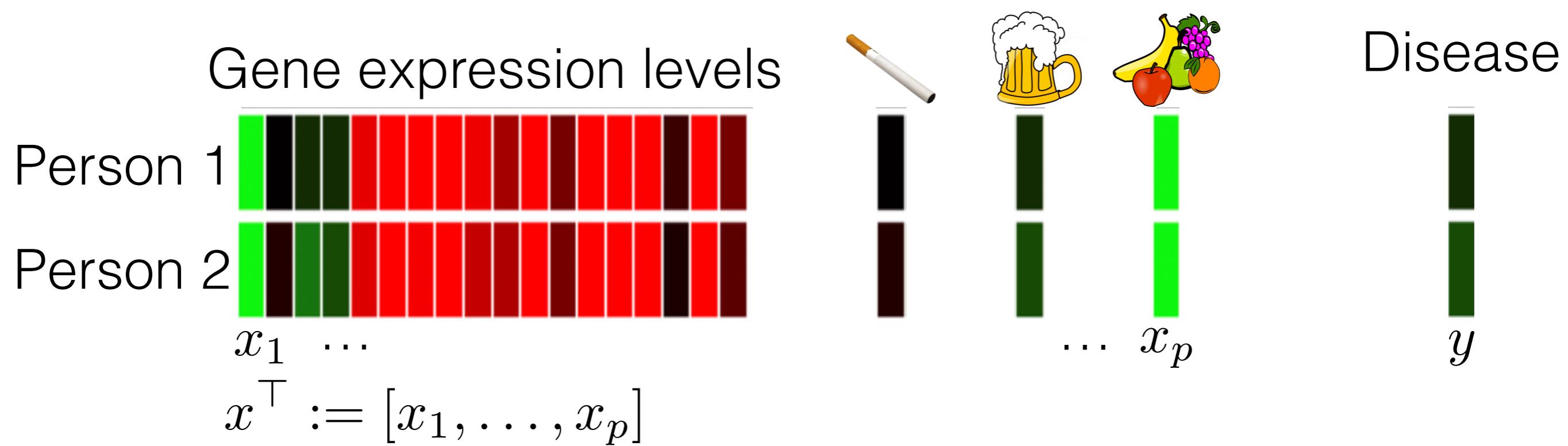
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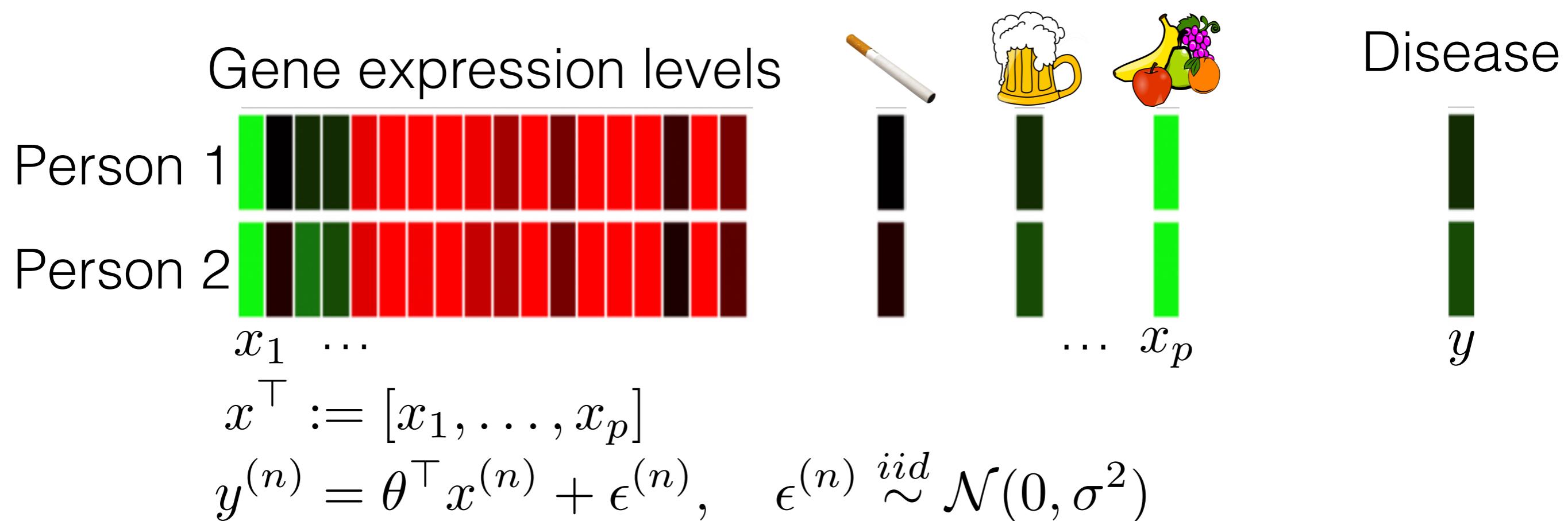
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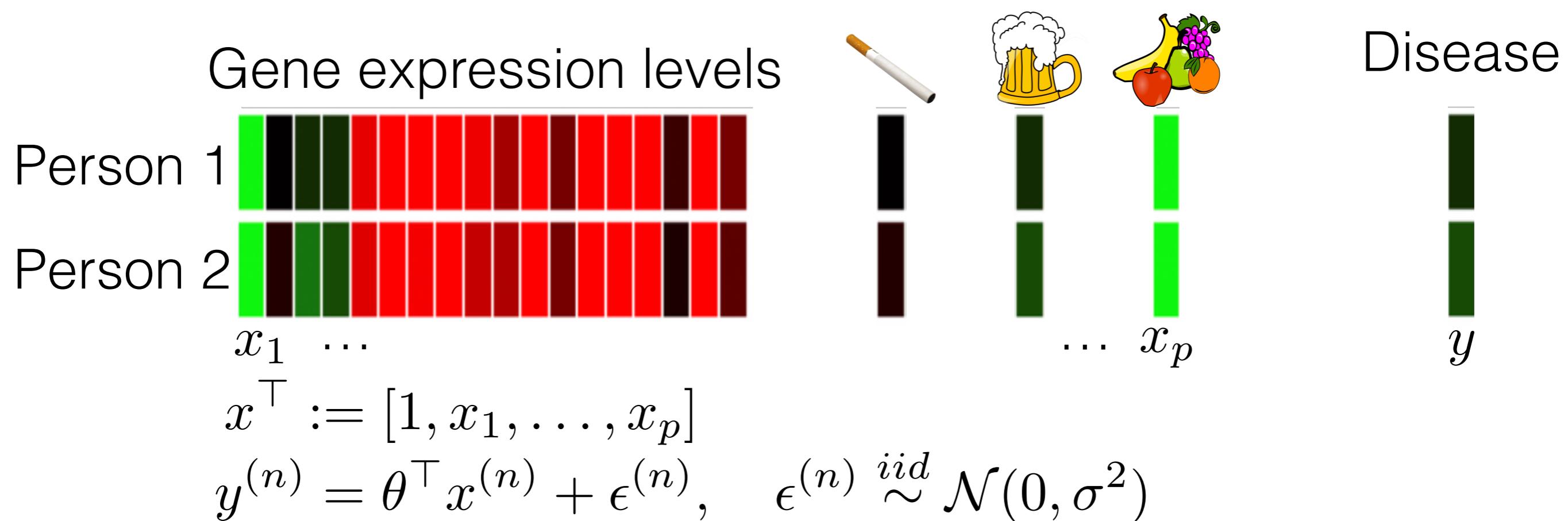
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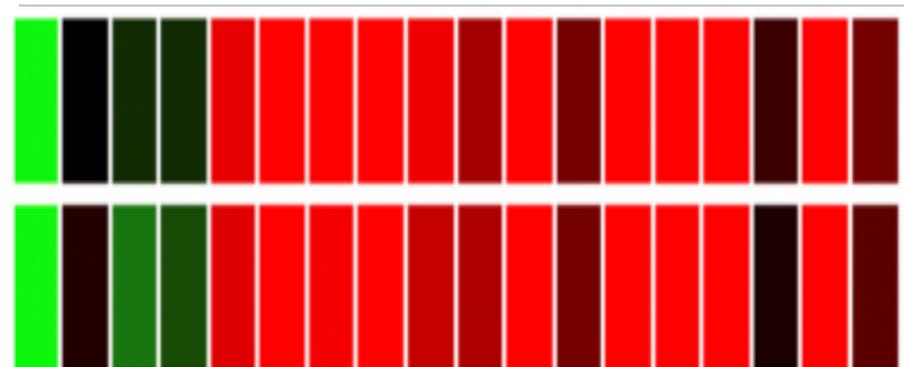
Discovering main and interaction effects



Discovering main and interaction effects

Gene expression levels

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Person 2



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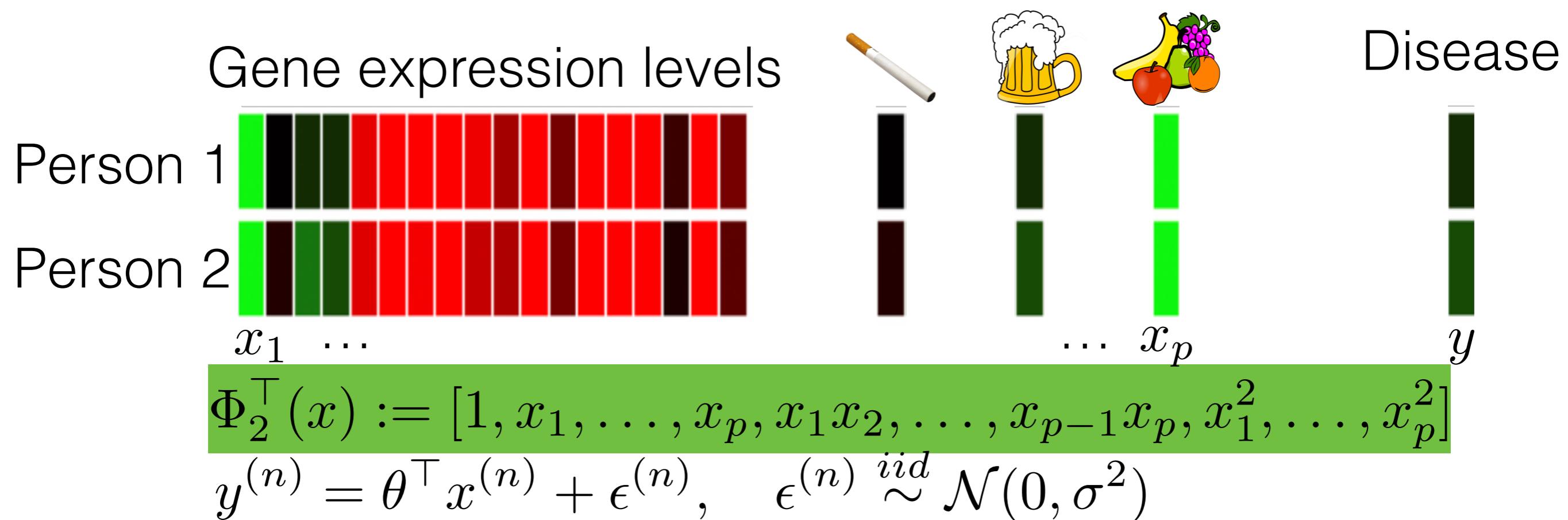
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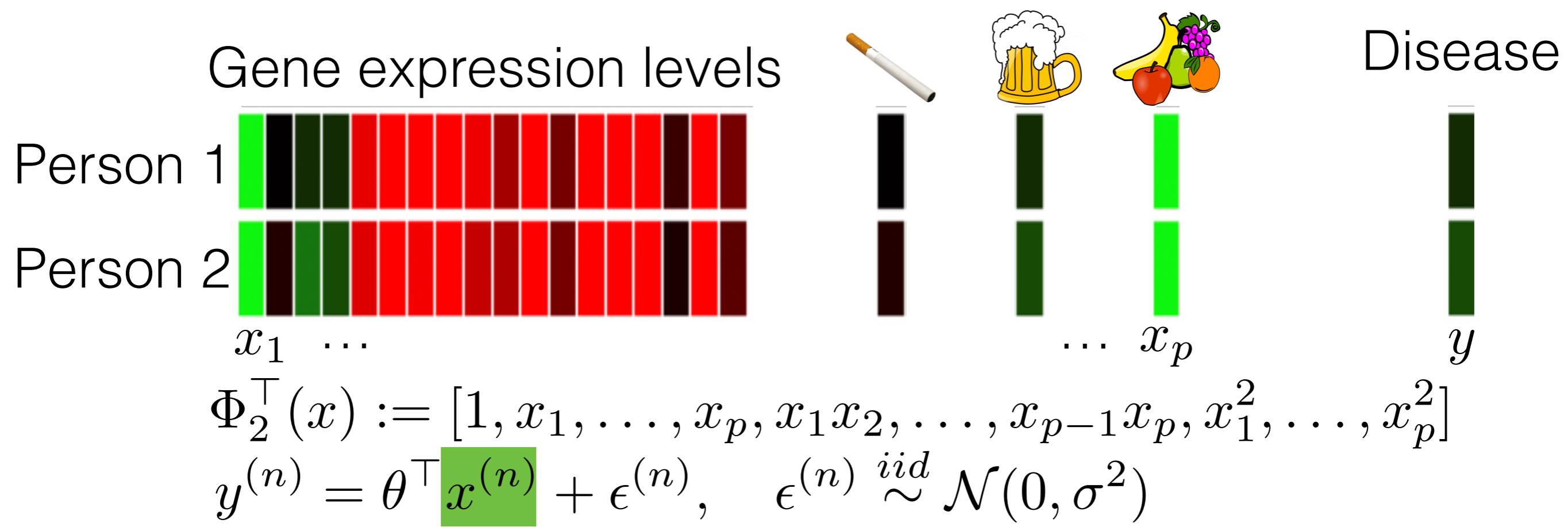
y

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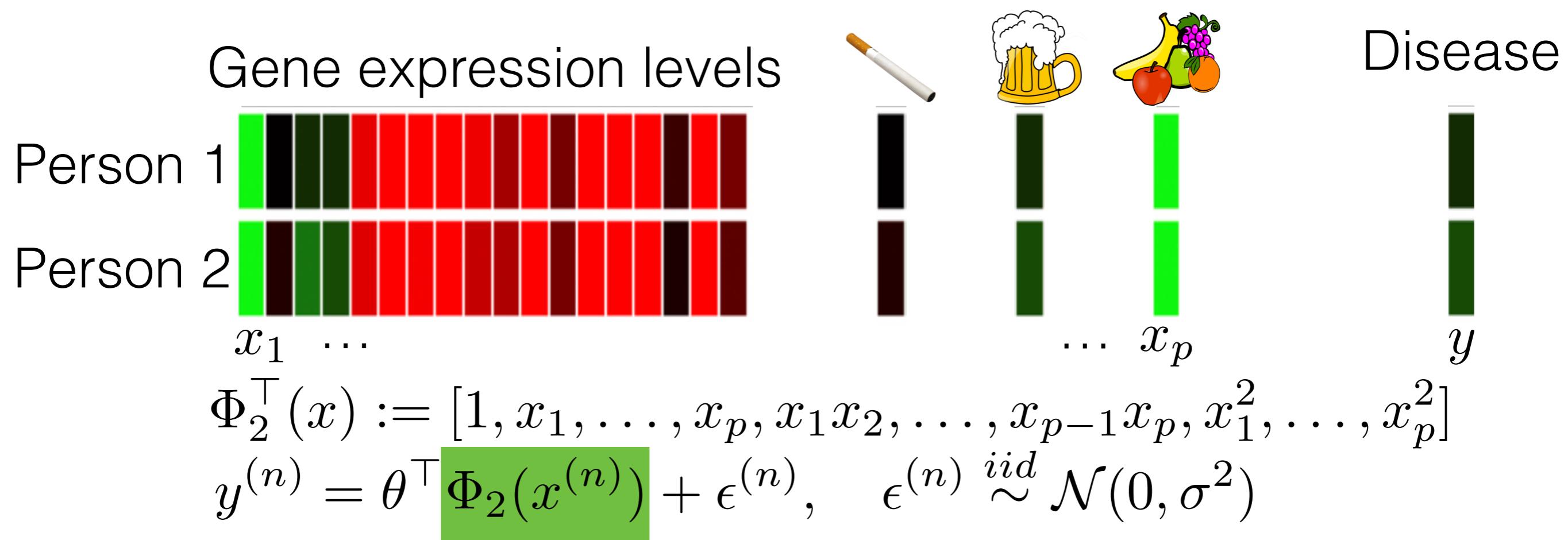
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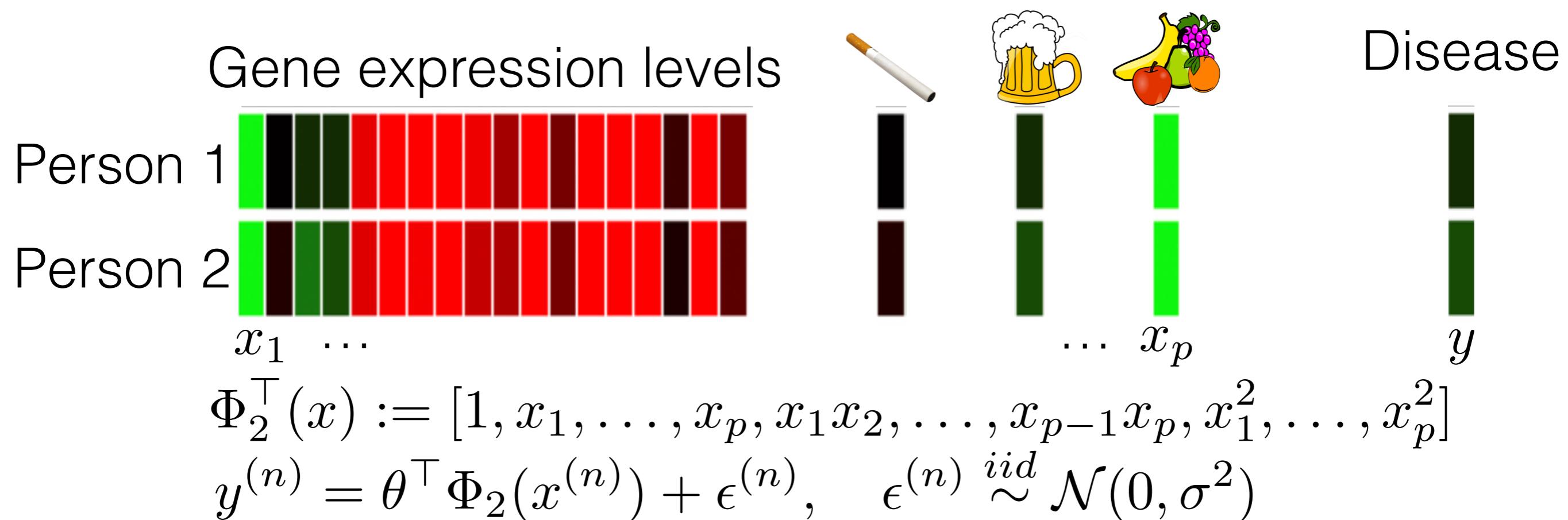
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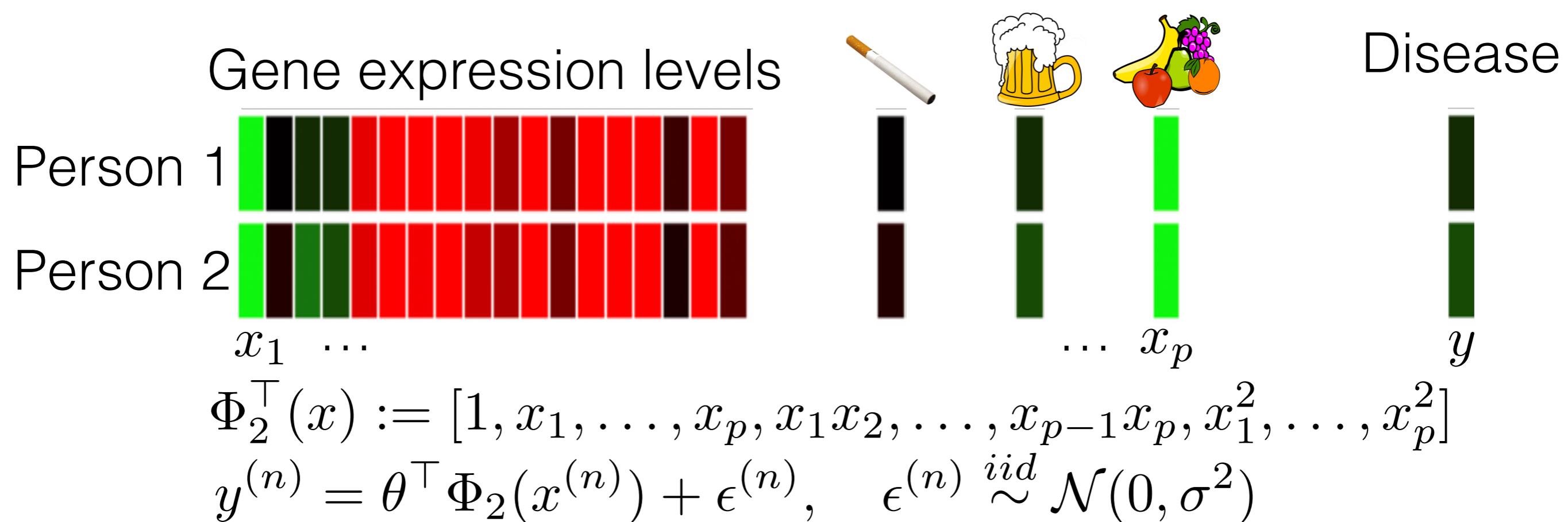
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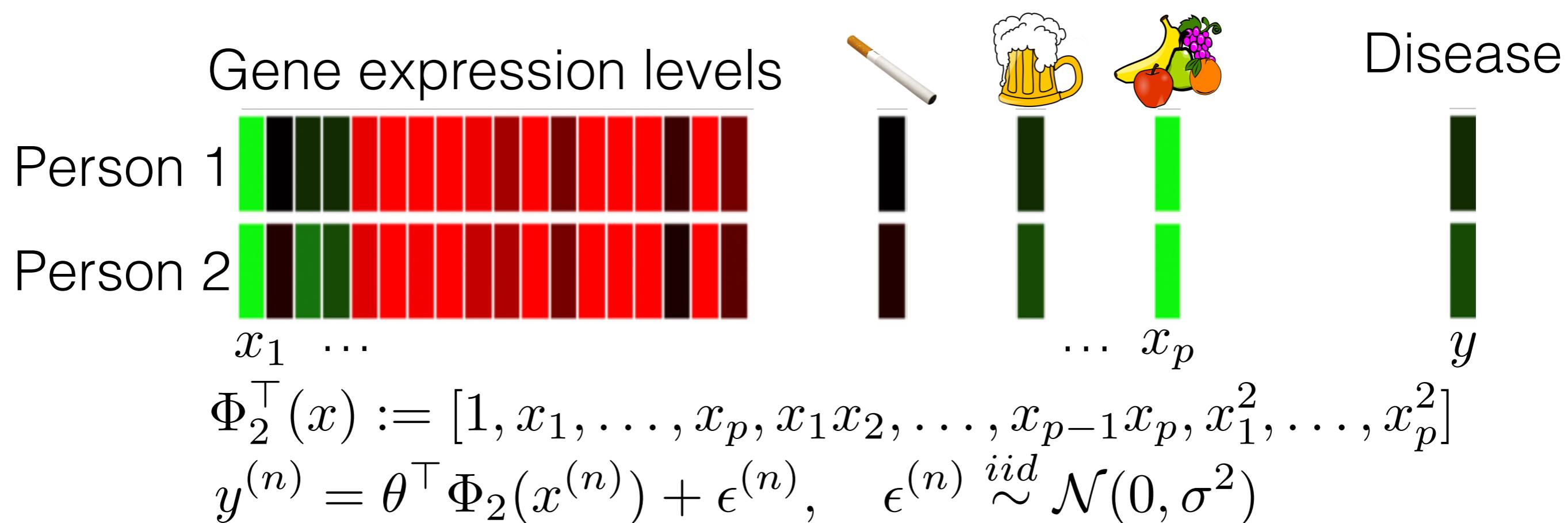


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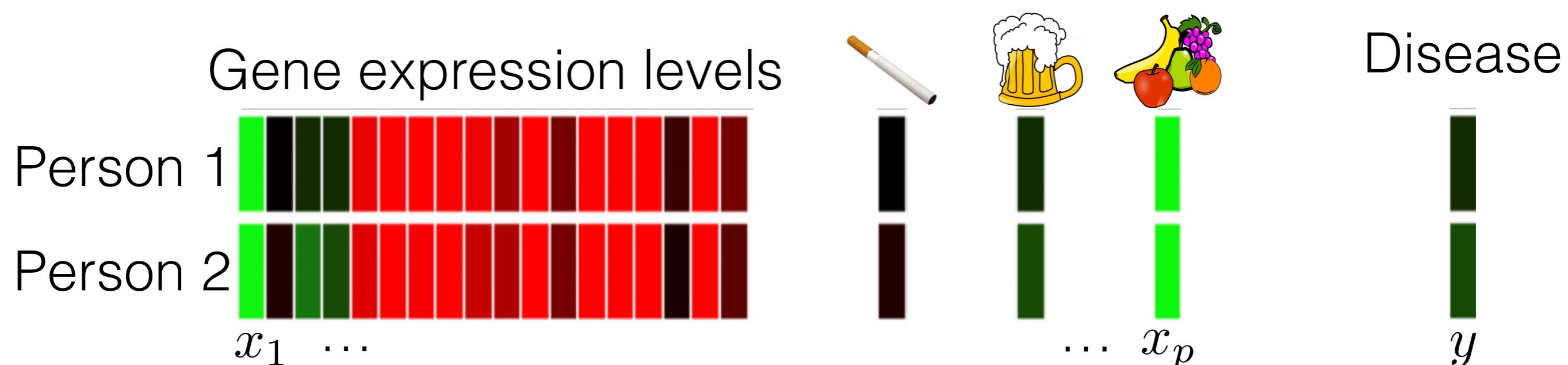
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Discovering main and interaction effects



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

Discovering main and interaction effects

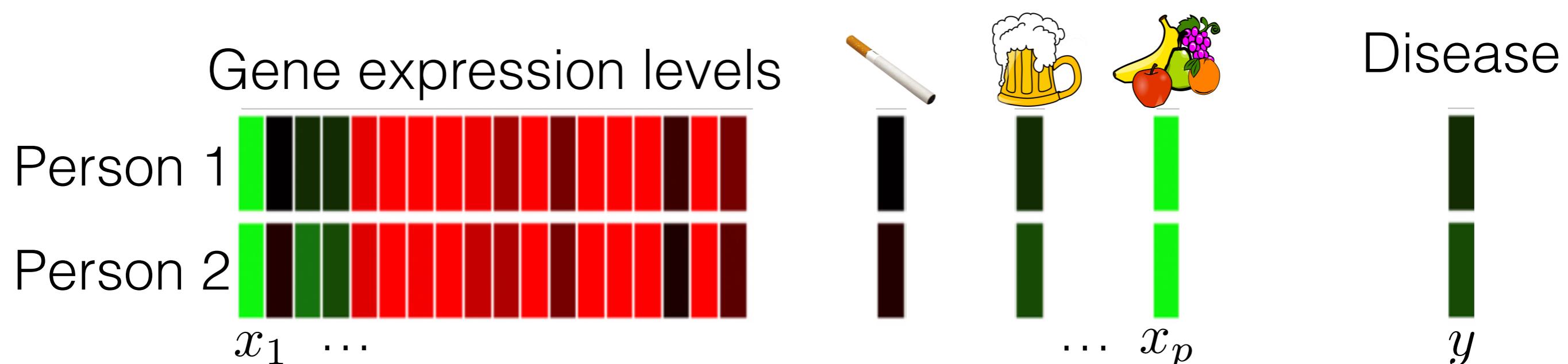


$$\Phi_2^\top(x) := [1, x_1, \dots, x_p, x_1 x_2, \dots, x_{p-1} x_p, x_1^2, \dots, x_p^2]$$

$$y^{(n)} = \theta^\top \Phi_2(x^{(n)}) + \epsilon^{(n)}, \quad \epsilon^{(n)} \stackrel{iid}{\sim} \mathcal{N}(0, \sigma^2)$$

- **Goal:** Parameter selection/estimation under assumptions:
 - *Sparsity:* most main effects are negligible (interpretable)

Discovering main and interaction effects

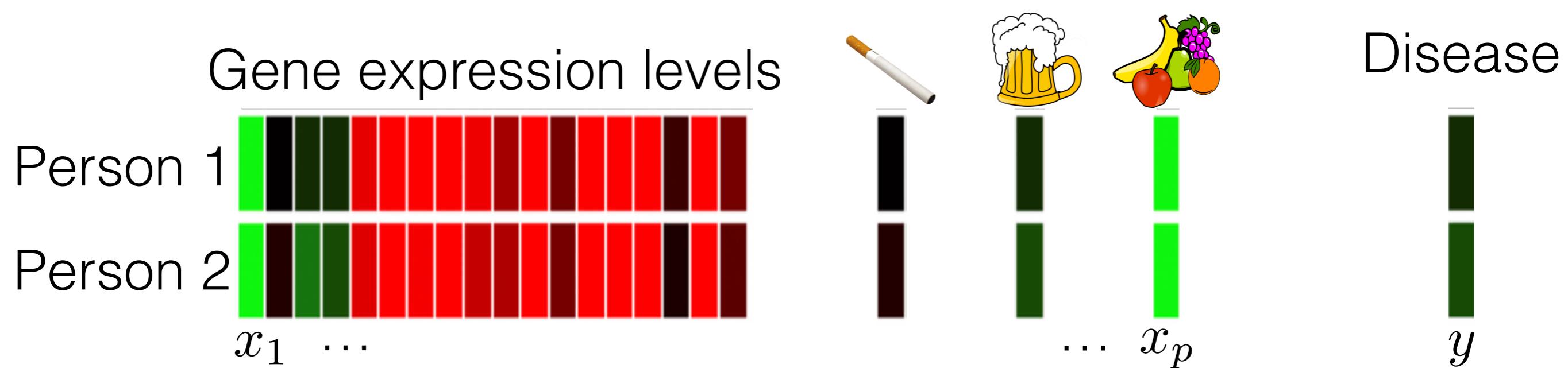


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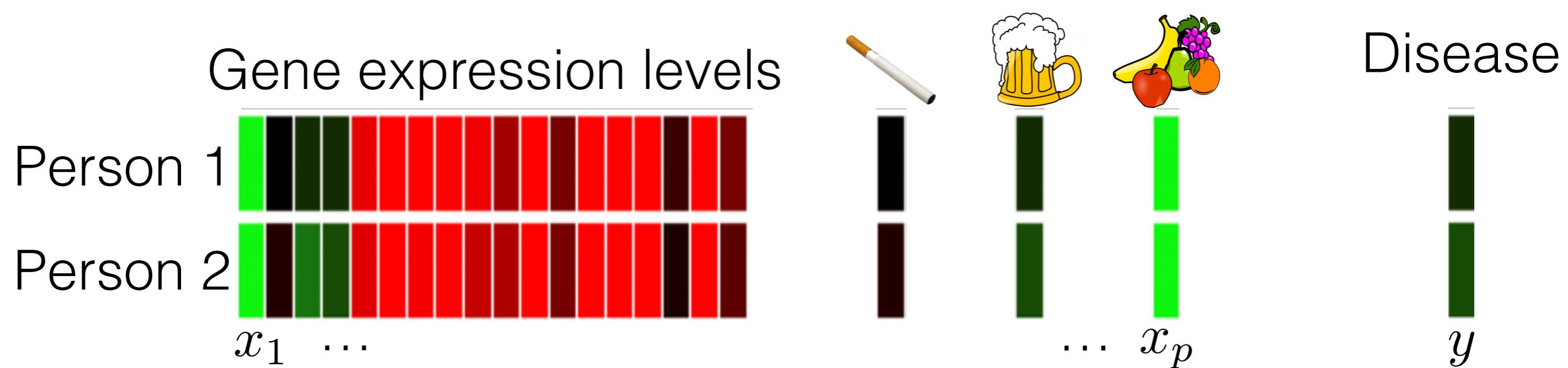
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- **Our solution:** using structure in covariates + sparsity assumptions to reduce to a problem *linear* in p

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Our approach

A Bayesian method: expert information, uncertainty quantification, regularization

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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

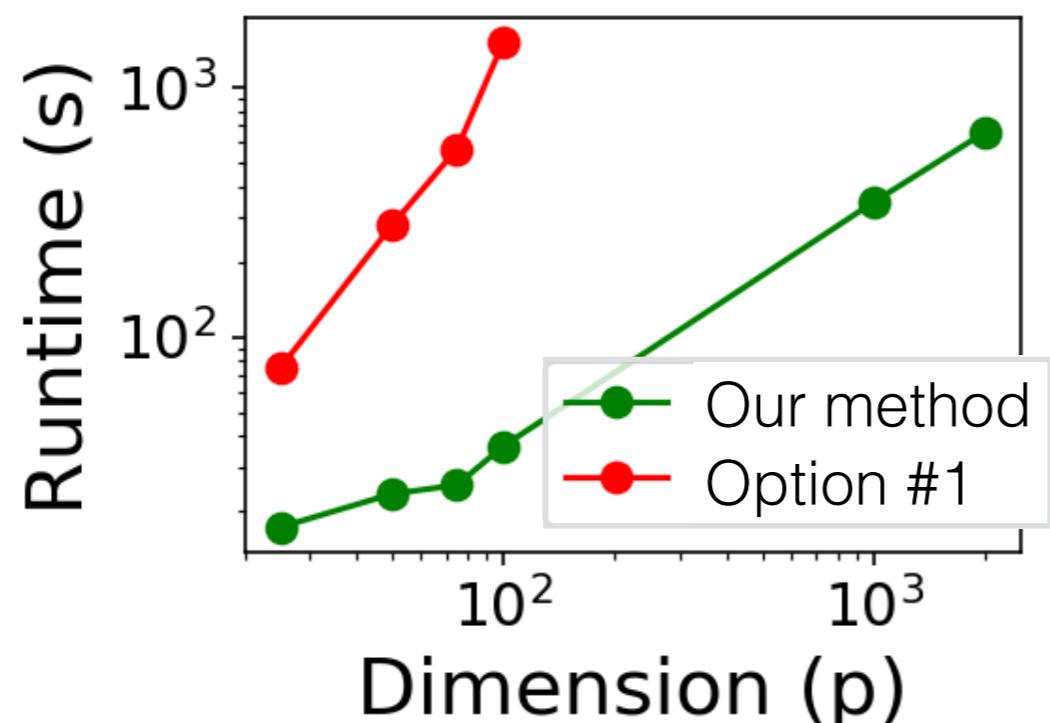
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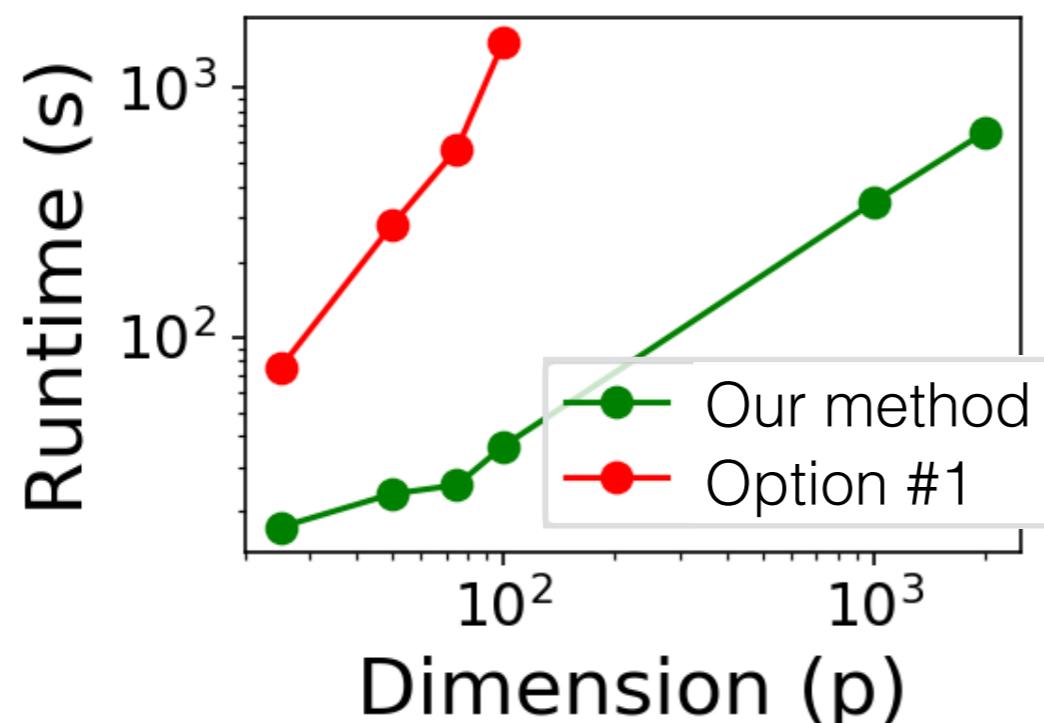
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- Mixing (1000 iters Stan):
 - Option #1: all $\hat{R} > 1.05$
 - Our method: all $\hat{R} < 1.05$

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$$X^\top X$$

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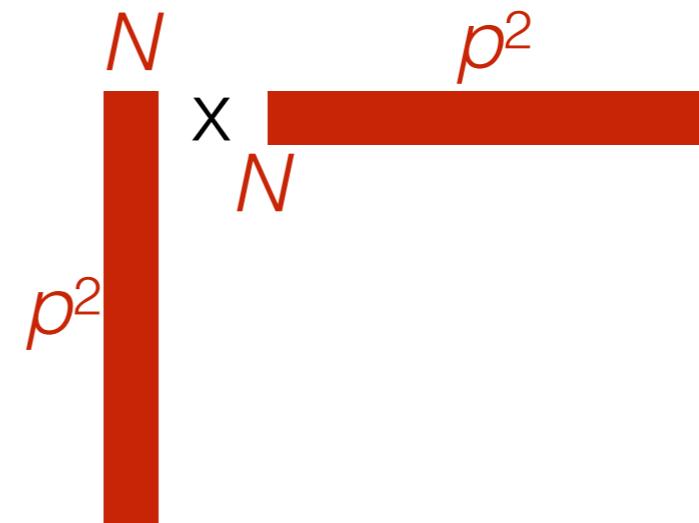
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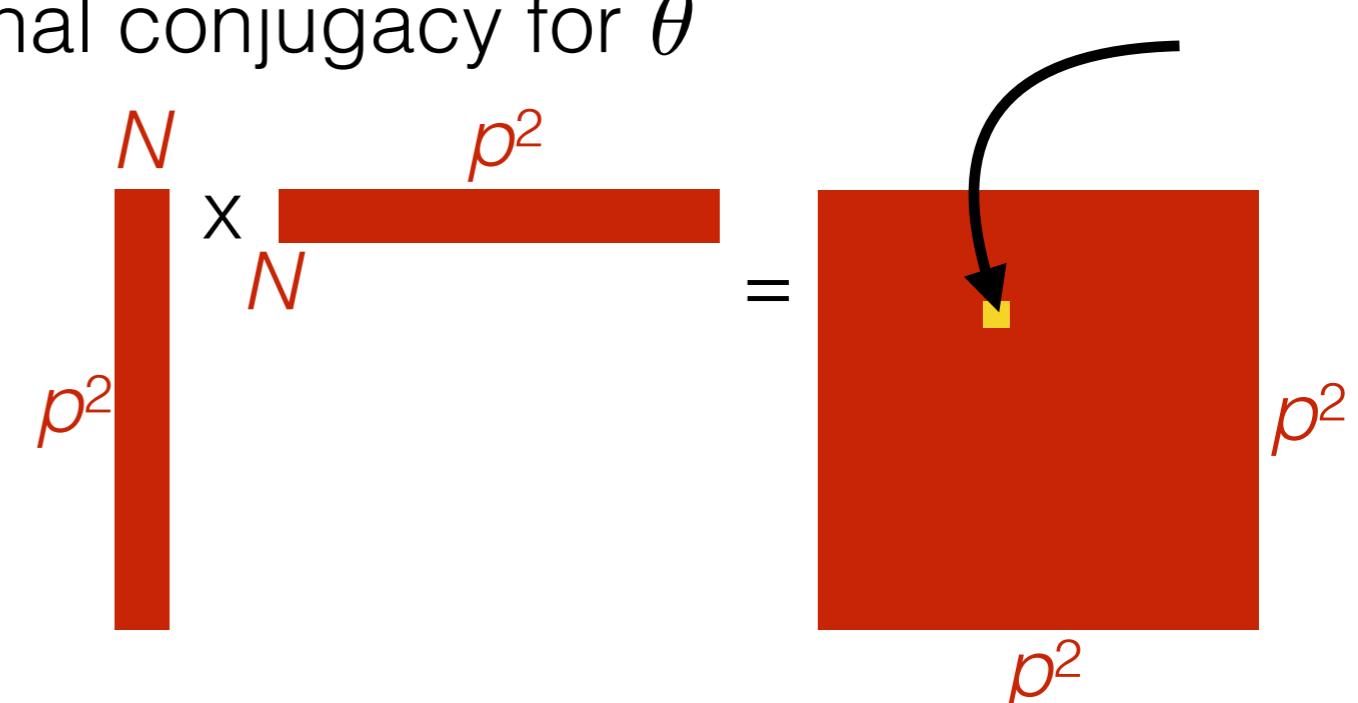
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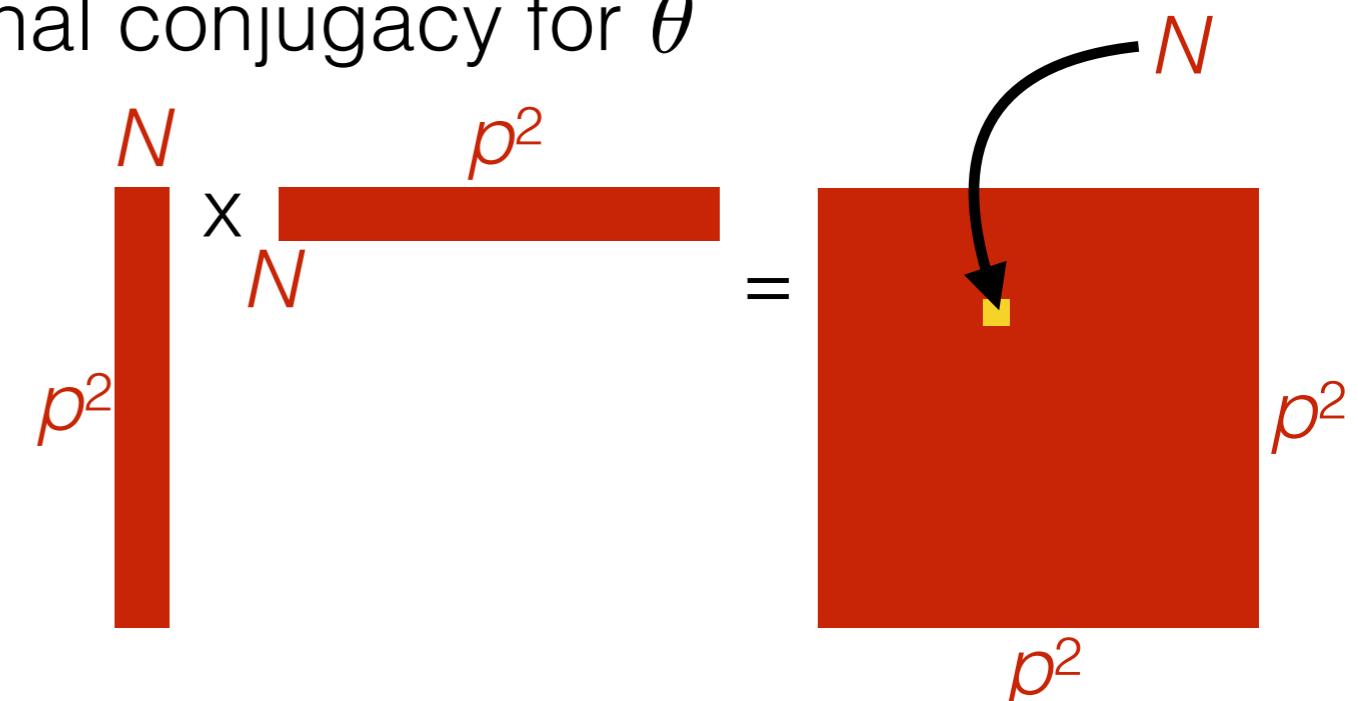
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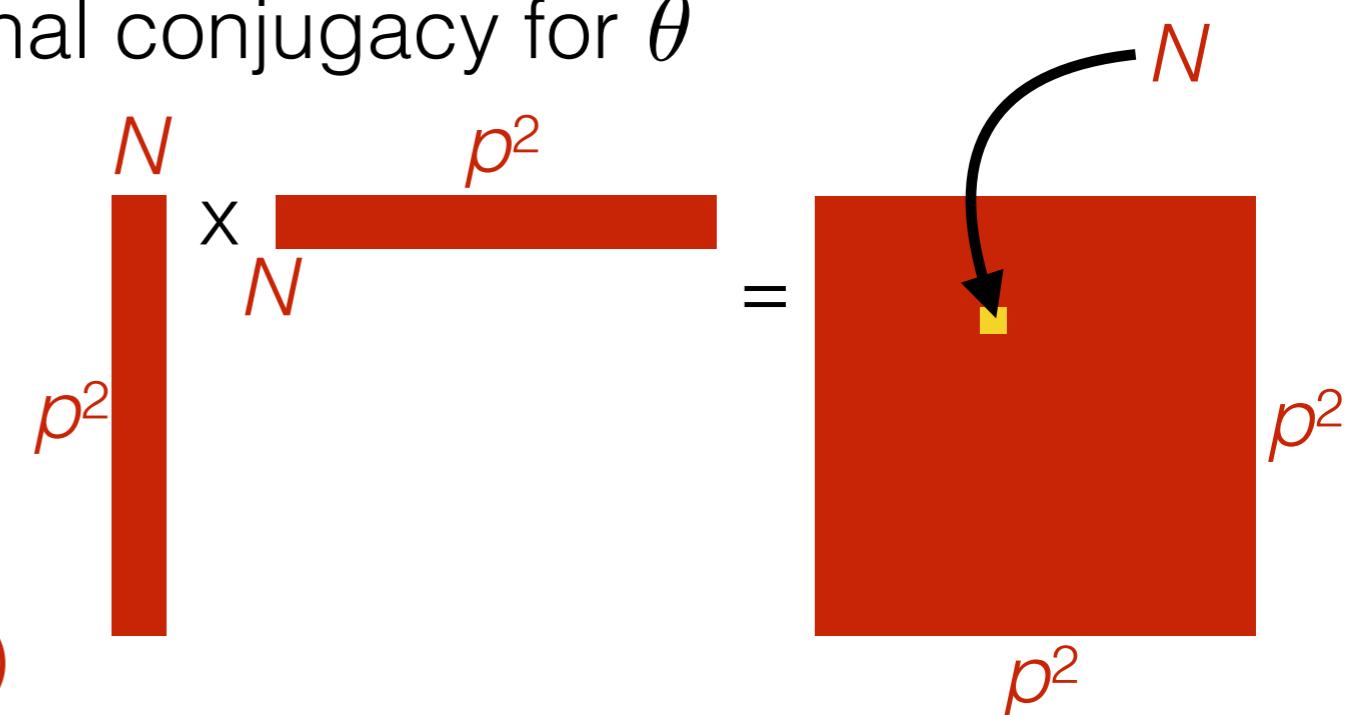
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- Naive time cost: $O(p^4N + p^6)$

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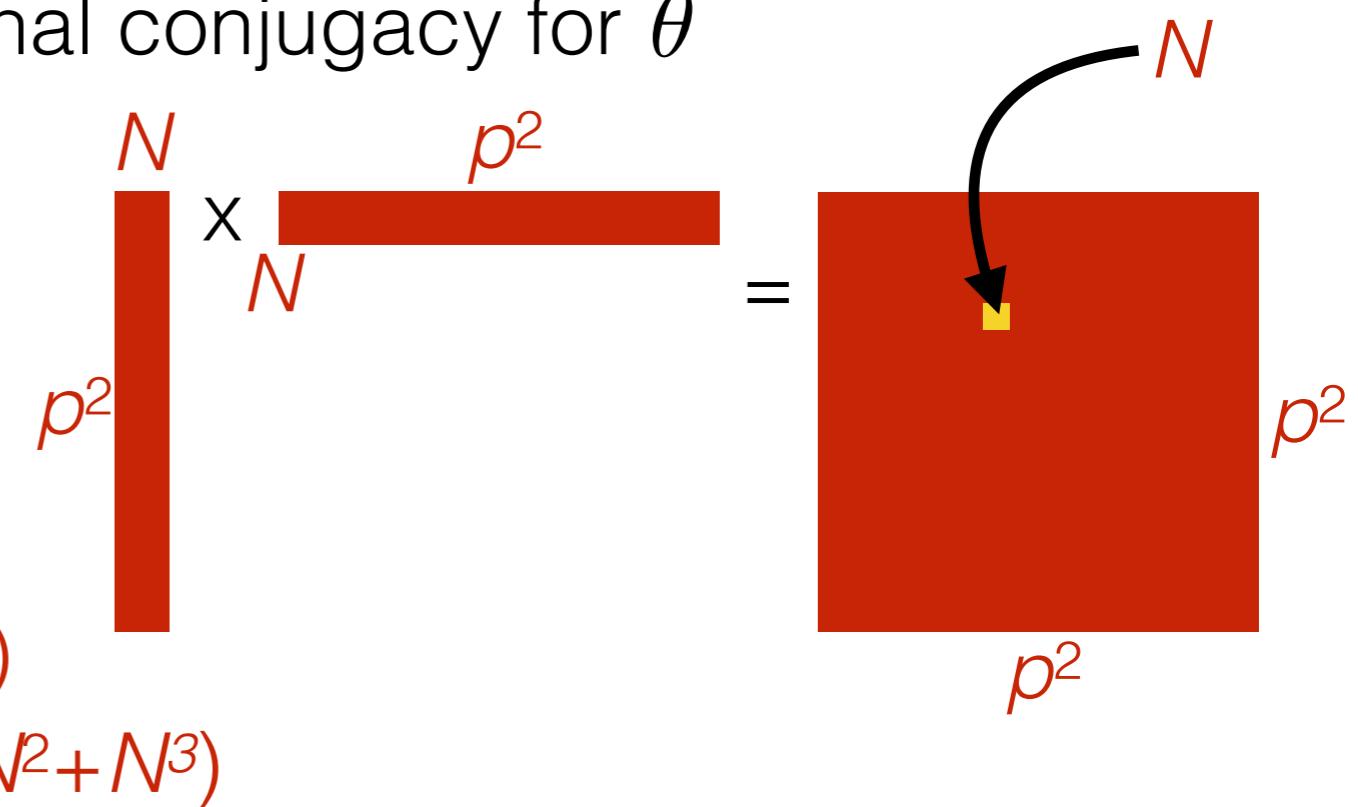
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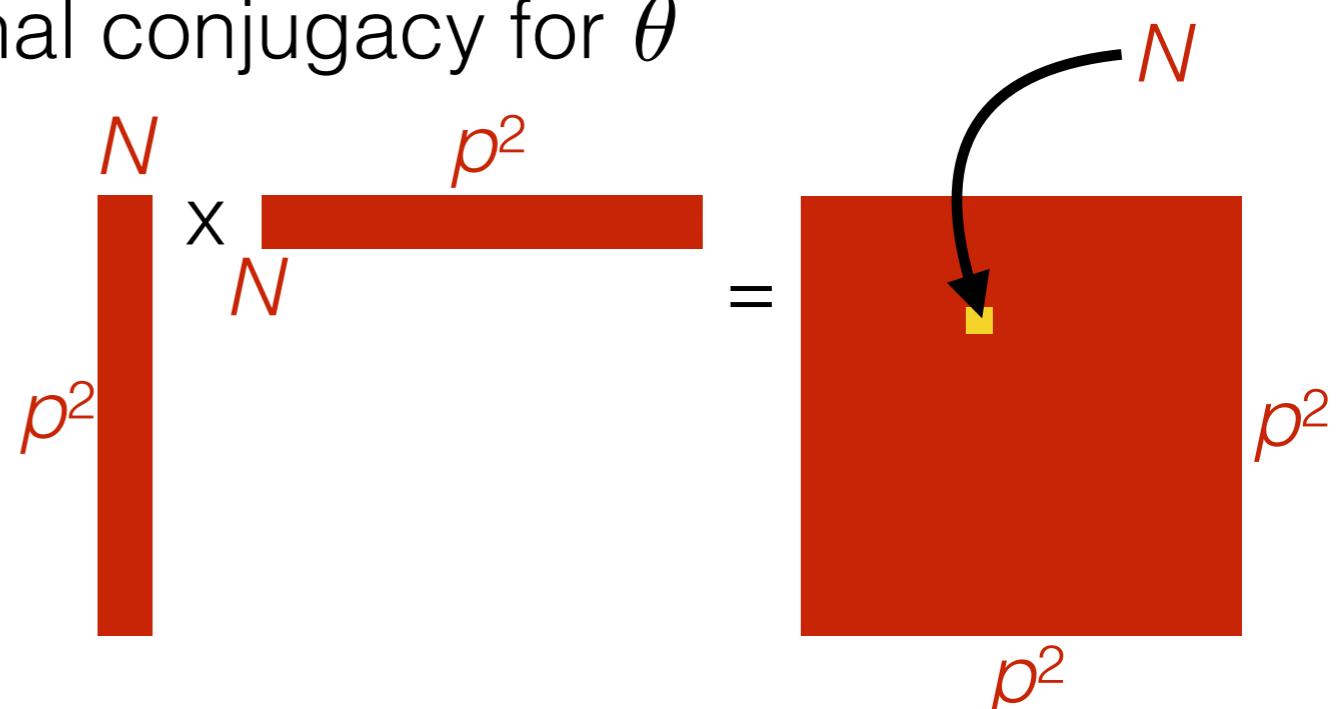
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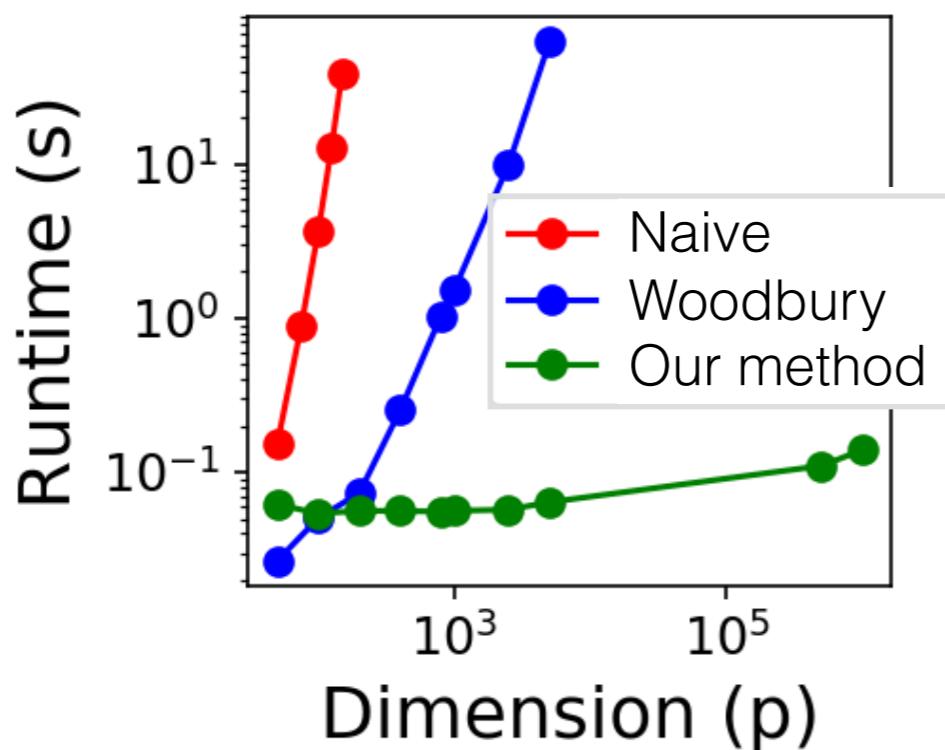
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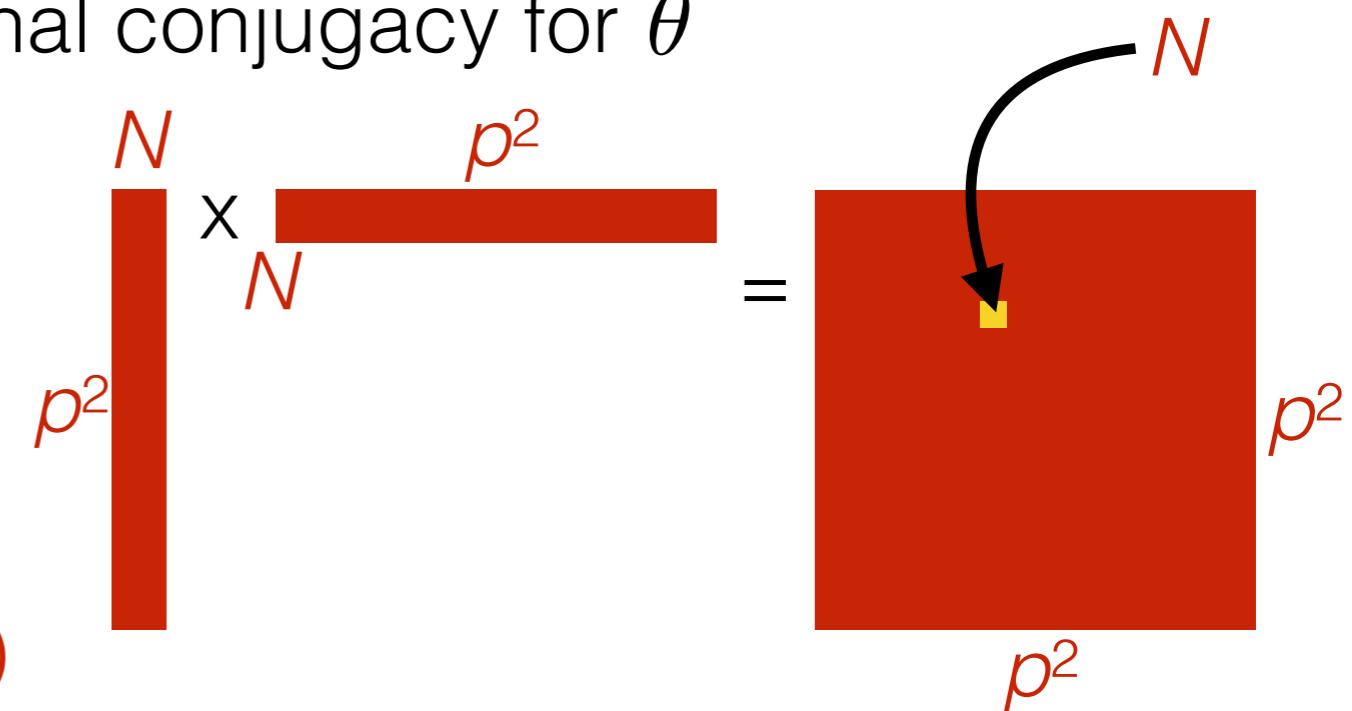
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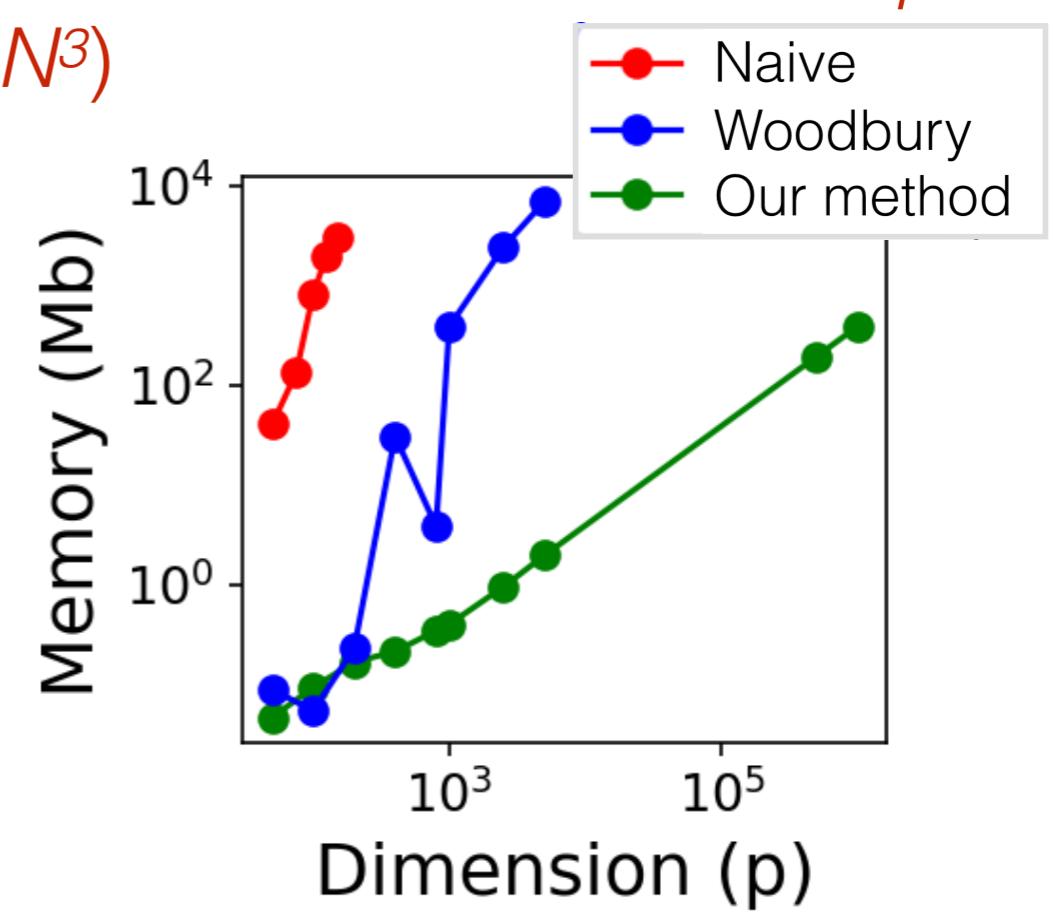
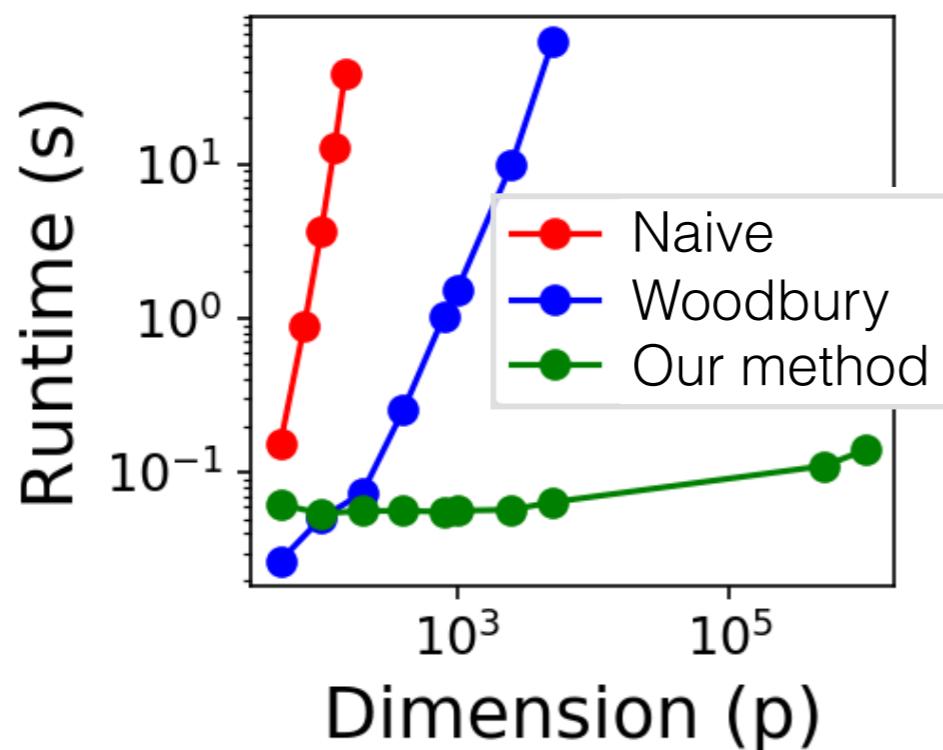
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Kernel Interaction Sampler vs. Naive MCMC

- Compute and invert

$$\Phi_2(X)^\top \Phi_2(X)$$

$X: N \times p$

$\Phi_2: N \times p^2$

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Kernel Interaction Sampler vs. Naive MCMC

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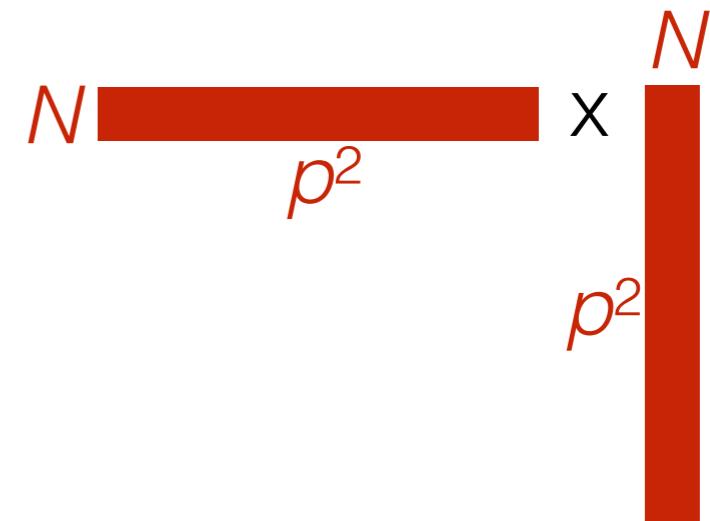
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$$N \overline{p^2}$$

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$$\Phi_2(X) \Phi_2(X)^T$$

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$$N \begin{matrix} \textcolor{red}{p^2} \\ \times \end{matrix} = \begin{matrix} \textcolor{red}{N} \\ \textcolor{red}{p^2} \end{matrix}$$

Kernel Interaction Sampler vs. Naive MCMC

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$$N \begin{array}{c} \\[-1ex] p^2 \end{array} \times \begin{array}{c} N \\[-1ex] p^2 \end{array} = \begin{array}{c} N \\[-1ex] N \end{array}$$

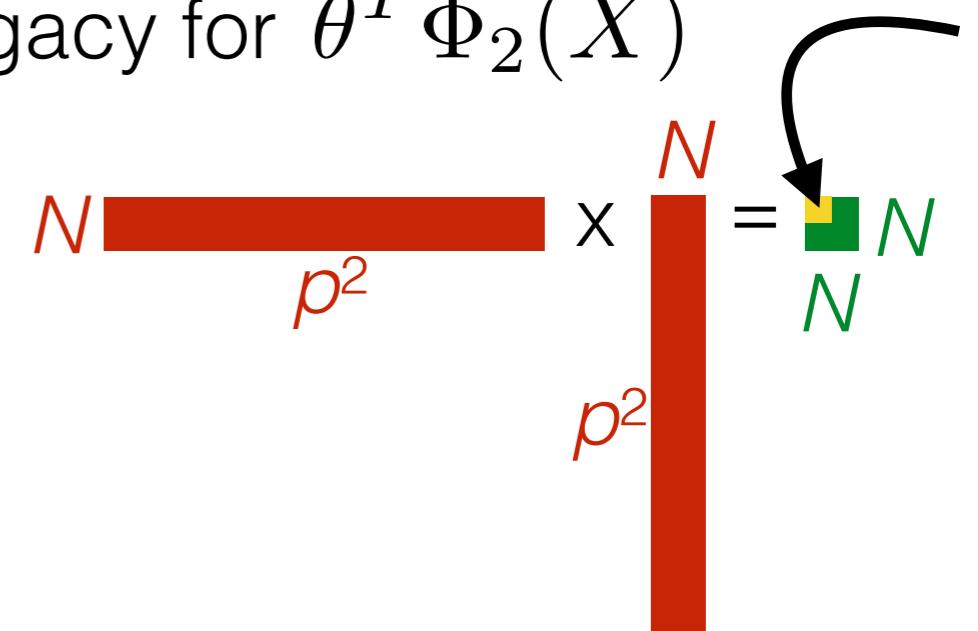
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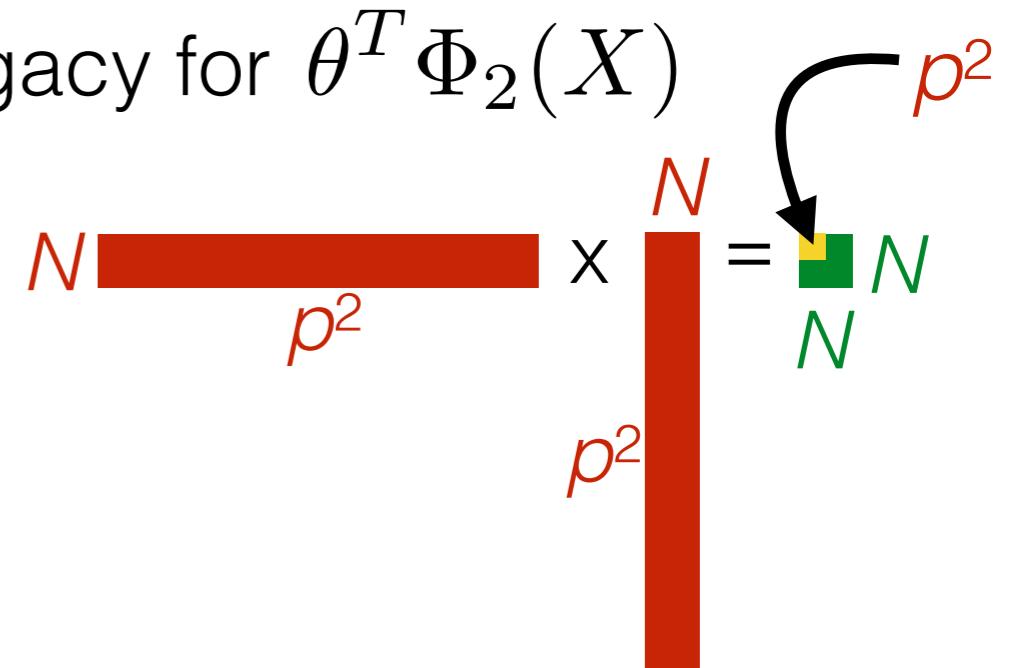
$\Phi_2: N \times p^2$

$$N \xrightarrow{p^2} \times \begin{matrix} N \\ p^2 \end{matrix} = \begin{matrix} N \\ N \end{matrix}$$


A diagram illustrating matrix multiplication. On the left, a red horizontal bar is labeled $N \xrightarrow{p^2}$. This is followed by a black multiplication sign (\times). To its right is a red vertical bar also labeled $N \xrightarrow{p^2}$. An arrow points from the top of the vertical bar to the right side of the multiplication sign. To the right of the multiplication sign is an equals sign ($=$). To the right of the equals sign is a green square containing the text $\begin{matrix} N \\ N \end{matrix}$.

Kernel Interaction Sampler vs. Naive MCMC

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Kernel Interaction Sampler vs. Naive MCMC

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The diagram illustrates a matrix multiplication operation. On the left, a red horizontal bar labeled N above and p^2 below is multiplied by a red vertical bar labeled N above and p^2 below. The result is a green square labeled N above and N below. A yellow box labeled p^2 is shown above the horizontal bar, and a black arrow points from it to the green square result.

Kernel Interaction Sampler vs. Naive MCMC

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Kernel Interaction Sampler vs. Naive MCMC

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A diagram illustrating matrix multiplication. On the left, a red horizontal bar labeled N above and p^2 below is multiplied by a red vertical bar labeled N to its right, also with p^2 written vertically below it. The result is a green square labeled N . A black arrow points from the p^2 label on the horizontal bar to the p^2 label on the vertical bar. A green bracket labeled p is positioned above the horizontal bar.

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A diagram illustrating matrix multiplication. On the left, a horizontal red bar is labeled N above p^2 . To its right is a vertical red bar also labeled N above p^2 . An equals sign follows. To the right of the equals sign is a horizontal red bar labeled N above N , and below it is a vertical red bar labeled N above N . A green arrow points from the top of the first vertical bar to the top of the second vertical bar.

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- Step C: Report just the k^2 strong-hierarchy interaction effects: takes $O(k^2)$ time

Roadmap

- Setup: Discovering main and interaction effects
- Our method
 - A Bayesian generative model
 - Fast inference
 - Fast reporting of results
- Experiments on simulated and real data

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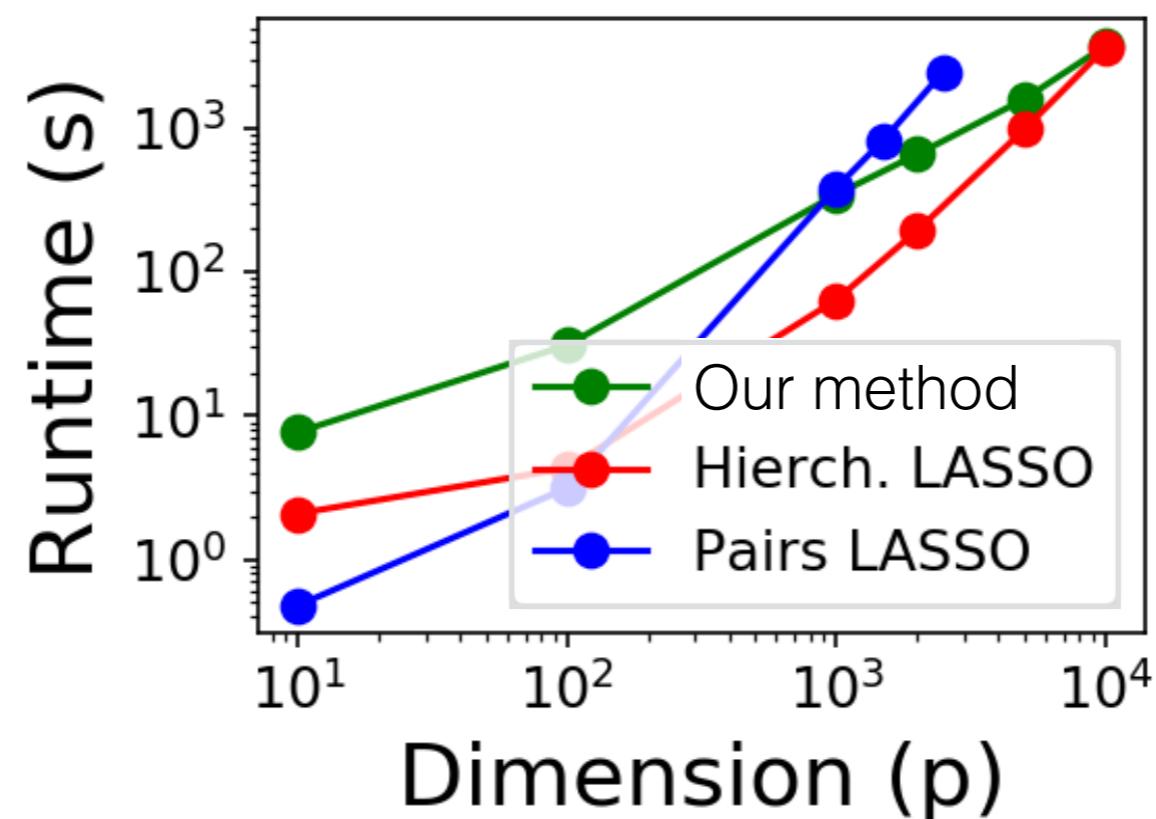
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- Competitive empirically for moderate p :



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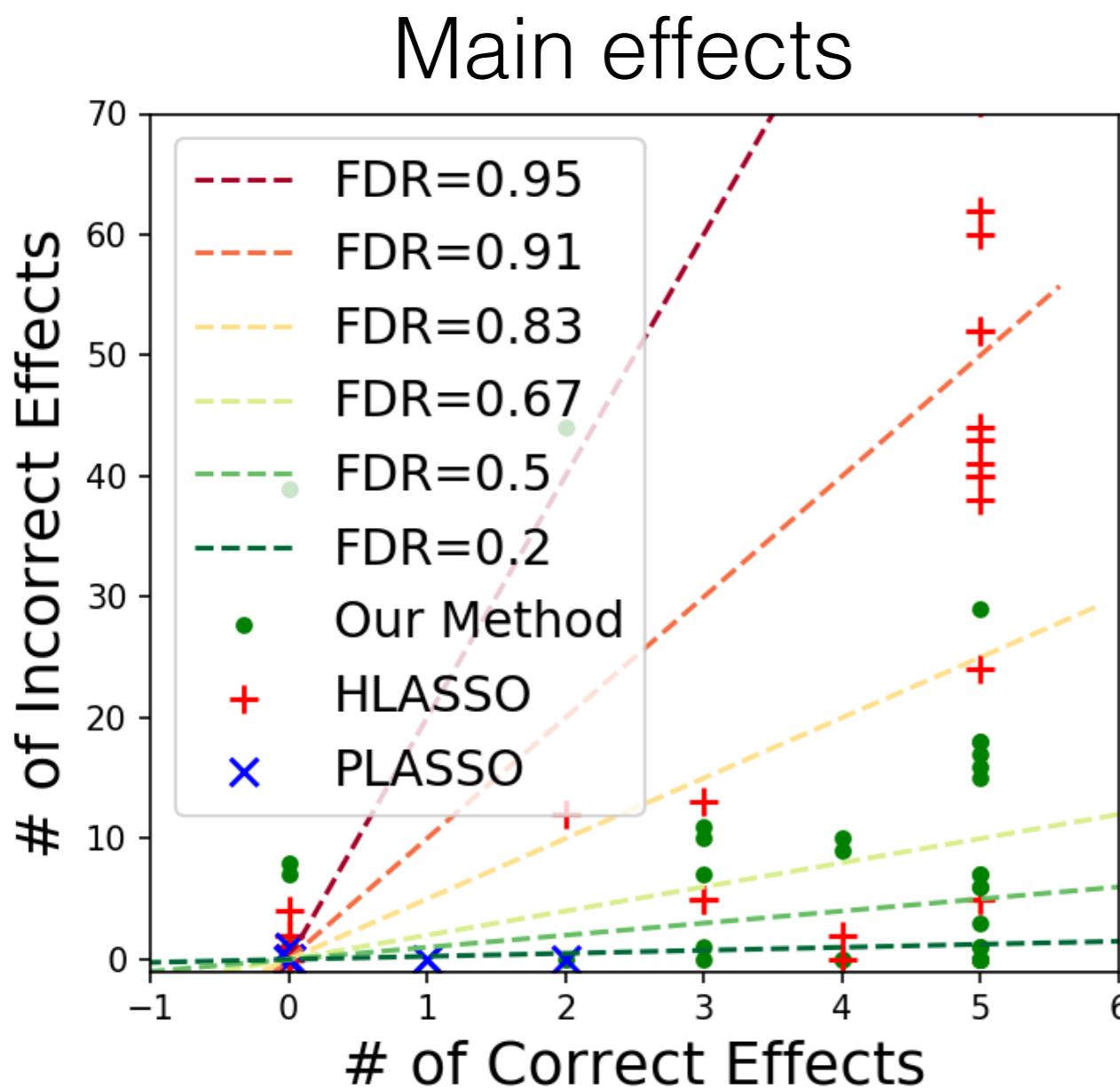
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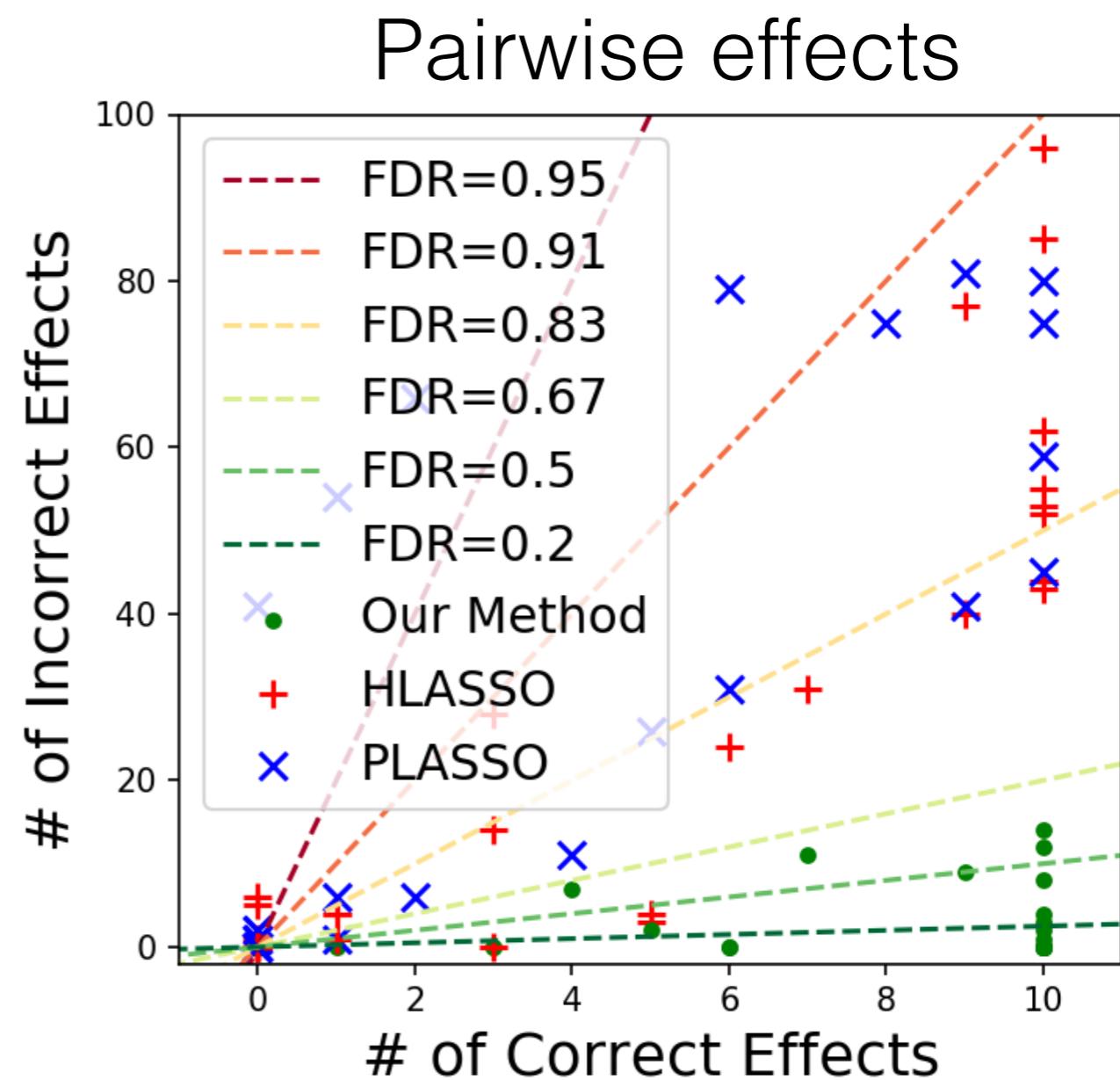
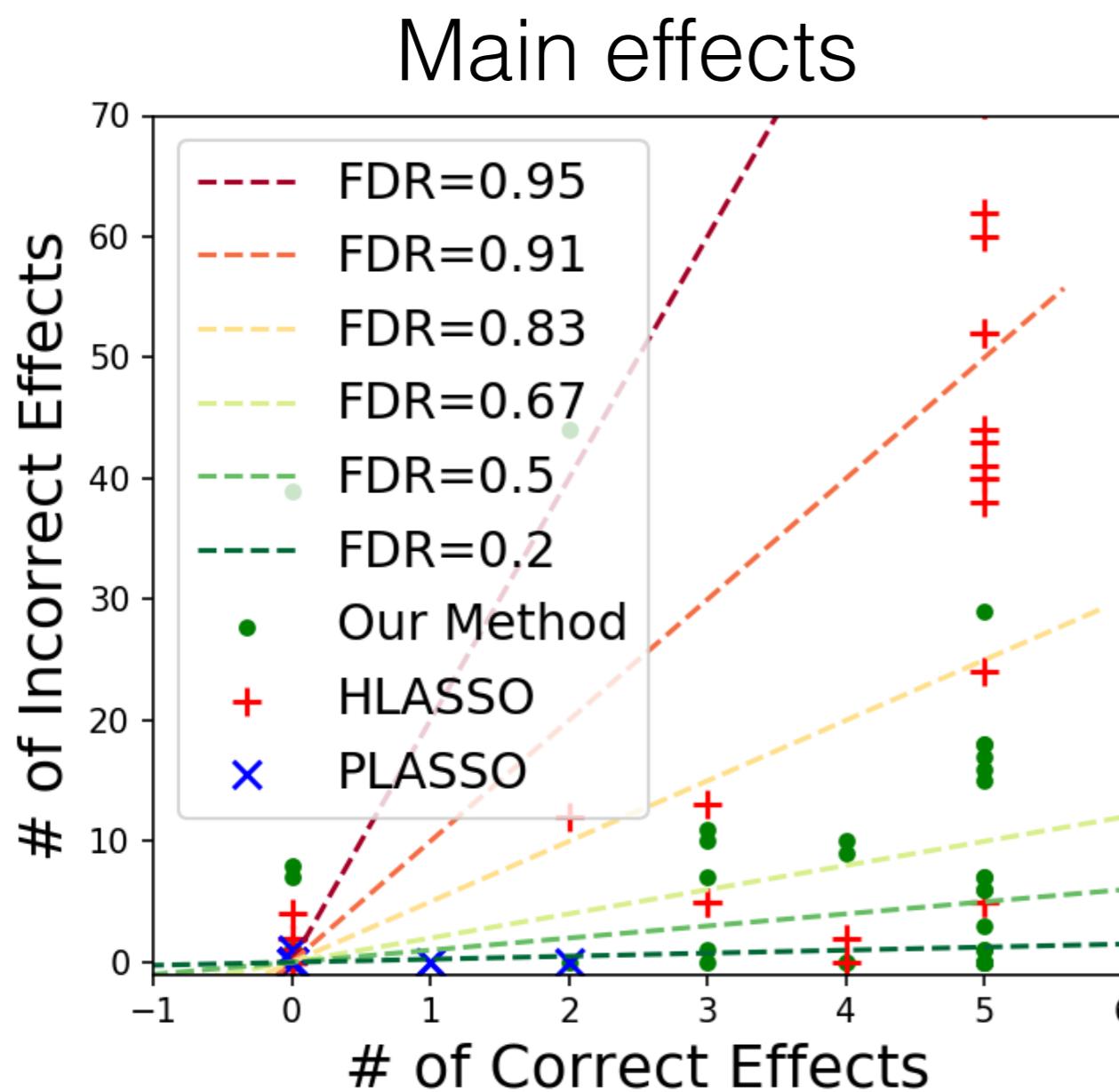
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METHOD	#MAIN	#PAIR
PLASSO	2 : 5	3 : 21

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METHOD	#MAIN	#PAIR
Our method	3 : 0	3 : 0
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HLASSO	3 : 19	3 : 18

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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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PLASSO	4 : 0	2 : 78
HLASSO	6 : 46	4 : 38

Conclusions

We provide: fast, accurate detection of pairwise interactions

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- Genetics (epistasis) application, etc

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Sparse Kernel Interaction Model (SKIM)

Likelihood

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

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

SKIM prior

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

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

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

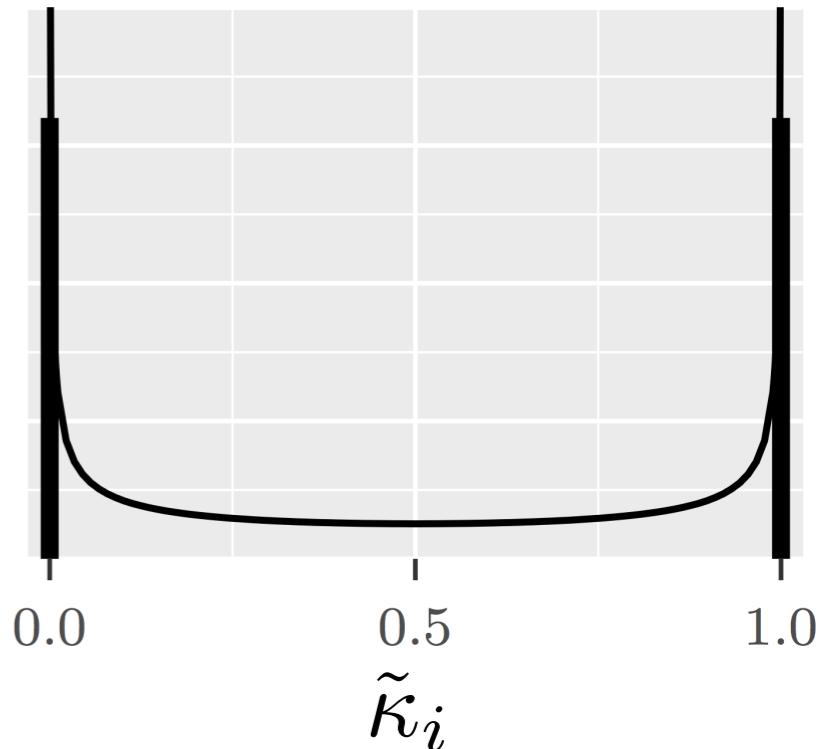
$$\theta_{x_i^2} \sim \mathcal{N}(0, \psi^2 (\tilde{\kappa}_i^2)^2)$$

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

$\tilde{\kappa}_i$: regularized horseshoe priors

m^2, ξ^2, ψ^2, c^2 : inverse gamma priors [Carvalho et al 2009; Piironen, Vehtari 2017]

[Piironen, Vehtari 2017]



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