

# Applications of Response Dimension Reduction in Large $p$ -Small $n$ Problems

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# Outline

- 1 Response Dimension Reduction Methodologies
- 2 Implementation along with Sample Size
- 3 Real Data Applications
- 4 Discussion



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# Response Dimension Reduction

- **Sufficient Dimension Reduction**

- Replace  $\mathbf{X} \in \mathbb{R}^p$  with lower dimensional projection  $\mathbf{P}_S \mathbf{X}$ , without losing information of  $\mathbf{Y} \mid \mathbf{X}$
- Find the orthogonal projection operator  $\mathbf{P}_S$ , such that

$$\mathbf{Y} \perp\!\!\!\perp \mathbf{X} \mid \mathbf{P}_S \mathbf{X}$$

- **Response Dimension Reduction**

- In multivariate regression of  $\mathbf{Y} \in \mathbb{R}^r \mid \mathbf{X} \in \mathbb{R}^p$  ( $r \geq 2$ ),  
**Sample size  $n$**  could be smaller than  $p$  or  $r \Rightarrow$  **Large  $p$ -Small  $n$  Problem**
  - Lead to exponential increase in the number of parameters  
(**curse of dimensionality**)
- Reduce the dimension of  $\mathbf{Y}$  without loss of information on  $E(\mathbf{Y} \mid \mathbf{X})$



# Non-parametric Method (YC-method)

## Linear Response Reduction (Yoo and Cook, 2008)

$$E(\mathbf{Y}|\mathbf{X}) = E\{\mathbf{P}_{\mathbf{L}(\Sigma_Y)}^T \mathbf{Y}|\mathbf{X}\}$$

where  $\mathbf{L} \in \mathbb{R}^{r \times q}$ ,  $q \leq r$ , and  $\mathbf{P}_{\mathbf{L}(\Sigma_Y)} = \mathbf{L}(\mathbf{L}^T \Sigma_Y \mathbf{L})^{-1} \mathbf{L}^T \Sigma_Y$  is an **orthogonal projection operator**.

## Conditional Response Reduction (Yoo and Cook, 2008)

$$E(\mathbf{Y}|\mathbf{X}) = E\{E(\mathbf{Y}|\mathbf{X}, \mathbf{K}^T \mathbf{Y})|\mathbf{X}\} = E\{E(\mathbf{Y}|\mathbf{K}^T \mathbf{Y})|\mathbf{X}\} = E\{g(\mathbf{K}^T \mathbf{Y})|\mathbf{X}\}$$

where  $\mathbf{K} \in \mathbb{R}^{r \times k}$ ,  $k \leq r$ ,  $\mathbf{K} \neq \mathbf{I}_r$ , and  $g(\cdot)$  represents an **unknown function**.

- Column spaces of  $\mathbf{L}$ ,  $\mathbf{K}$  : *Response dimension reduction subspace*
- $\mathcal{S}(\mathbf{K}) \subseteq \mathcal{S}(\mathbf{L})$ , and  $\mathcal{S}(\mathbf{K}) = \mathcal{S}(\mathbf{L})$  iff  $E(\mathbf{Y}|\mathbf{K}^T \mathbf{Y} = a)$  is linear in  $a$
- To estimate  $\mathbf{L}$  and  $\mathbf{K}$ ,  $\Sigma_Y^{-1} \text{cov}(\mathbf{Y}, \mathbf{X}^T) \Sigma_X^{-1}$  is needed
  - $\Sigma_X = \text{cov}(\mathbf{X})$  and  $\Sigma_Y = \text{cov}(\mathbf{Y})$  are positive-definite matrices



# Principal Response Reduction

## Principal Response Reduction (Yoo, 2018)

Assume both  $E(\mathbf{Y})$  and  $E(\mathbf{X})$  are zero without loss of generality:

$$\mathbf{Y} = \mathbf{\Gamma} \boldsymbol{\nu}_x + \boldsymbol{\varepsilon}$$

where  $d \leq r$ ,  $\mathbf{\Gamma} \in \mathbb{R}^{r \times d}$  is an **orthogonal** matrix,  $\boldsymbol{\varepsilon} \sim N(0, \boldsymbol{\Sigma})$ , and  $\text{cov}(\boldsymbol{\nu}_x, \boldsymbol{\varepsilon}) = 0$ .  $\boldsymbol{\nu}_x$  is a  $d$ -dimensional **unknown function** of  $\mathbf{X}$ , and  $\boldsymbol{\Sigma}_x \boldsymbol{\nu}_x = 0$ .

- $\mathcal{S}(\mathbf{\Gamma})$  is invariant, and reduces subspace for  $\boldsymbol{\Sigma}$
  - $\boldsymbol{\Sigma} = \mathbf{\Gamma} \boldsymbol{\Omega} \mathbf{\Gamma}^T + \mathbf{\Gamma}_0 \boldsymbol{\Omega}_0 \mathbf{\Gamma}_0^T$ 
    - $\mathbf{\Gamma}_0 \in \mathbb{R}^{r \times (r-d)}$ ,  $\mathbf{\Gamma}_0^T \mathbf{\Gamma}_0 = \mathbf{I}_{r-d}$ ,  $\mathbf{\Gamma}_0^T \mathbf{\Gamma} = 0$ ,  $\boldsymbol{\Omega} = \mathbf{\Gamma}^T \boldsymbol{\Sigma} \mathbf{\Gamma}$ , and  $\boldsymbol{\Omega}_0 = \mathbf{\Gamma}_0^T \boldsymbol{\Sigma} \mathbf{\Gamma}_0$
  - $E(\mathbf{Y}|\mathbf{X}) = E(\mathbf{P}_{\mathbf{\Gamma}(\boldsymbol{\Sigma}_y)}^T \mathbf{Y}|\mathbf{X})$  holds
  - MLE for  $\mathbf{\Gamma}$  is derived from the 1st  $d$  largest eigenvectors of  $\hat{\boldsymbol{\Sigma}}_y$ 
    - $\mathcal{L}_{\text{PRR}}(\mathbf{\Gamma}_0, \boldsymbol{\Upsilon}) = -\frac{n}{2} \log |\mathbf{\Gamma}_0^T \hat{\boldsymbol{\Sigma}}_y \mathbf{\Gamma}_0| - \frac{n}{2} \log |\boldsymbol{\Upsilon}|$ , where  $\boldsymbol{\Upsilon} \in \mathbb{S}^{r \times r}$  stand for  $\boldsymbol{\Omega}$
- $\Rightarrow$  No need for inverse matrix
- However, in **PRR**,  $\mathbf{\Gamma}$  does not consider  $\mathbf{X}$ , only utilizes  $\mathbf{Y}$



# Principal Fitted Response Reduction

## Principal Fitted Response Reduction (Yoo, 2018)

To incorporate  $\mathbf{X}$ , assume  $\boldsymbol{\nu}_x = \boldsymbol{\psi} \mathbf{f}_x$ ,

$$\mathbf{Y} = \boldsymbol{\Gamma} \boldsymbol{\psi} \mathbf{f}_x + \boldsymbol{\varepsilon}$$

where  $\boldsymbol{\psi} \in \mathbb{R}^{d \times q}$  is an unknown matrix,  $\mathbf{f}_x$  is a  $q$ -dimension **known vector function** of  $\mathbf{X}$ , and  $\boldsymbol{\Sigma}_x \mathbf{f}_x = 0$ .

- $\mathbf{Y}$ :  $n \times r$  response data matrix
- $\mathbf{F}$ :  $n \times q$  matrix stacking  $\mathbf{f}_x^T$
- $\mathbf{P}_F = \mathbf{F}(\mathbf{F}^T \mathbf{F})^{-1} \mathbf{F}^T$
- $\hat{\boldsymbol{\Sigma}}_{\text{fit}} = \mathbf{Y}^T \mathbf{P}_F \mathbf{Y} / n$  and  $\hat{\boldsymbol{\Sigma}}_{\text{res}} = \hat{\boldsymbol{\Sigma}}_y - \hat{\boldsymbol{\Sigma}}_{\text{fit}}$
- MLE for  $\boldsymbol{\Gamma}$  does not have a closed-form solution
  - $\mathcal{L}_{\text{PFRR}}(\boldsymbol{\Gamma}, \boldsymbol{\Gamma}_0) = -\frac{n}{2} \log |\boldsymbol{\Gamma}_0^T \hat{\boldsymbol{\Sigma}}_y \boldsymbol{\Gamma}_0| - \frac{n}{2} \log |\boldsymbol{\Gamma}^T \hat{\boldsymbol{\Sigma}}_{\text{res}} \boldsymbol{\Gamma}|$
  - $\boldsymbol{\Gamma}$  is influenced by both  $\hat{\boldsymbol{\Sigma}}_y$  and  $\hat{\boldsymbol{\Sigma}}_{\text{res}}$

$\Rightarrow$  Only needs inverse of  $\mathbf{F}^T \mathbf{F}$



# Unstructured Principal Fitted Response Reduction

## Unstructured Principal Fitted Response Reduction (Yoo, 2019)

Assume that  $\epsilon \sim N(0, \Sigma > 0)$ , and  $\text{cov}(\nu_x, \epsilon) = 0$ :

$$\mathbf{Y} = \Gamma \psi \mathbf{f}_x + \epsilon$$

- $\Sigma = \Gamma \Omega \Gamma^T + \Gamma_0 \Omega_0 \Gamma_0^T$  does not need anymore
- $\mathcal{S}(\Sigma \Gamma) \subseteq \mathcal{S}(\Gamma)$  iff  $\mathcal{S}(\Sigma_y \Gamma) \subseteq \mathcal{S}(\Gamma)$   
 $\Rightarrow E(\mathbf{Y}|\mathbf{X}) = E(\mathbf{P}_{\Gamma(\Sigma_y)}^T \mathbf{Y}|\mathbf{X})$  if  $\mathcal{S}(\Gamma)$  is invariant for  $\Sigma_y$

- $\hat{\Sigma} = \hat{\Sigma}_{\text{res}} + \hat{\Sigma}_{\text{res}}^{1/2} \hat{\mathbf{V}} \hat{\mathbf{K}}_d \hat{\mathbf{V}}^T \hat{\Sigma}_{\text{res}}^{1/2} = \hat{\Sigma}_{\text{res}}^{1/2} (\mathbf{I}_r + \hat{\mathbf{V}} \hat{\mathbf{K}}_d \hat{\mathbf{V}}^T) \hat{\Sigma}_{\text{res}}^{1/2}$
- $\hat{\mathcal{S}}(\Gamma) = \hat{\Sigma}^{1/2} \mathcal{S}_d(\mathbf{B}) = \hat{\Sigma}_{\text{res}}^{1/2} \mathcal{S}_d(\mathbf{B}_{\text{res}})$ 
  - $\mathbf{B}_d$ : 1st  $d$  eigenvectors of  $\mathbf{B}$
  - $\mathbf{B} = \hat{\Sigma}^{-1/2} \hat{\Sigma}_{\text{fit}} \hat{\Sigma}^{-1/2}$
  - $\hat{\Lambda} = (\hat{\lambda}_1, \dots, \hat{\lambda}_q)$ : Eigenvalues of  $\mathbf{B}_{\text{res}}$
  - $\hat{\mathbf{K}}_d = \text{diag}(0, \dots, 0, \hat{\lambda}_{d+1}, \dots, \hat{\lambda}_q)$
  - $\mathcal{S}_d(\mathbf{B})$ : Column subspace of  $\mathbf{B}_d$
  - $\mathbf{B}_{\text{res}} = \hat{\Sigma}_{\text{res}}^{-1/2} \hat{\Sigma}_{\text{fit}} \hat{\Sigma}_{\text{res}}^{-1/2}$
  - $\hat{\mathbf{V}} = (\hat{\gamma}_1, \dots, \hat{\gamma}_q)$ : Eigenvectors of  $\mathbf{B}_{\text{res}}$

$\Rightarrow$  Inverse of  $\Sigma_{\text{res}}$  and  $\mathbf{F}^T \mathbf{F}$  (from  $\Sigma_{\text{fit}}$ ) is needed





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# Implementation along with Sample Size

$p$ : dimension of predictor,  $r$ : dimension of response,  $n$ : sample size

- **YC-method** (Non-parametric method)
  - Requires inverse matrices of  $\hat{\Sigma}_x$  and  $\hat{\Sigma}_y$   
 $\Rightarrow p < n, r < n$
- **PRR** (Principal Response Reduction)
  - Does not require inverse matrix  
 $\Rightarrow$  No constraints for  $p$ ,  $r$ , and  $n$
- **PFRR** (Principal Fitted Response Reduction)
  - Requires inverse matrix of  $F^T F$   
 $\Rightarrow p < n$
- **UPFRR** (Unstructured Principal Fitted Response Reduction)
  - Requires inverse matrices of  $F^T F$  and  $\hat{\Sigma}_{\text{res}}$   
 $\Rightarrow p < n, r < n$



# Implementation along with Sample Size

**Table 1. Feasible response dimension reduction methods** according to  $p$ ,  $r$  and  $n$

	Relation between $p$ , $r$ , $n$	Feasible methods
<b>case 1</b>	$\max(p, r) < n$	YC-method, PRR, PFRR, UPFRR
<b>case 2</b>	$p \geq n$ , but $r < n$	PRR
<b>case 3</b>	$p < n$ , but $r \geq n$	PRR, PFRR
<b>case 4</b>	$\min(p, r) \geq n$	PRR

- **case 2:**  $r < n \leq p$ 
  - Reducing  $p$  with **multivariate seeded** dimension reduction (Yoo and Im, 2014)  
⇒ Enable YC-method, PFRR, UPFRR
- **case 3:**  $p < n \leq r$ 
  - Reducing  $r$  through **PRR** or **PFRR**  
⇒ Enable YC-method, UPFRR
- **case 4:**  $n \leq \min(p, r)$ 
  1. Reducing  $r$  through **PRR**
  2. Reducing  $p$  with **multivariate seeded** dimension reduction  
⇒ Enable YC-method, PFRR, UPFRR



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# Real data analysis I (case 2: $p \geq n$ , $r < n$ )

## Near-infrared (NIR) Spectroscopy of Biscuit Doughs data

- **cookie** dataset from the **seedCCA** package (Kim et al., 2021)
  - **X** ( $p = 256$ ): **wavelengths** spanning from 1380 to 2400nm at 4nm intervals
  - **Y** ( $r = 4$ ): **fat** ( $Y_1$ ), **sucrose** ( $Y_2$ ), **dry flour** ( $Y_3$ ), **water** ( $Y_4$ )
  - $n_{\text{train}} = 39$ ,  $n_{\text{test}} = 31$  ( $n \leq p$ )  $\Rightarrow$  **Require reducing  $p$**

$\Rightarrow \mathbf{X}_{\text{train}}: 39 \times 256$ ,  $\mathbf{X}_{\text{test}}: 31 \times 256$ ,  $\mathbf{Y}_{\text{train}}: 39 \times 4$ ,  $\mathbf{Y}_{\text{test}}: 31 \times 4$

- Based on the **multivariate seeded** dimension reduction,  
**X** ( $p = 256$ )  $\rightarrow$  **Rx** ( $p' = 4$ )

- **Rx**<sub>train</sub>:  $39 \times 4$ , **Rx**<sub>test</sub>:  $31 \times 4$  ( $p' < n$ )

$\Rightarrow$  **UPFRR**, **PFRR**, and **PRR** are applied



# Real data analysis I (case 2: $p \geq n$ , $r < n$ )

Table 2. UPFRR and PFRR Results for `cookie` data

Comparison	Stat	df	p-value
0D vs $\geq$ 1D	340.9	32	<0.0001
1D vs $\geq$ 2D	159.4	21	<0.0001
2D vs $\geq$ 3D	27.39	12	0.0068
3D vs $\geq$ 4D	9.508	5	0.0904

(a) UPFRR Test Summary

Comparison	Stat	df	p-value
0D vs $\geq$ 1D	340.9	32	<0.0001
1D vs $\geq$ 2D	196.1	24	<0.0001
2D vs $\geq$ 3D	63.80	16	<0.0001
3D vs $\geq$ 4D	11.38	8	0.1809

(b) PFRR Test Summary

- For  $(R_x, Y)$ , both **UPFRR** and **PFRR** suggest reducing **Y** to 3 dimensions (5% significance level)

Table 3. Cumulative Variance of 1-4 Dimensions with Each RDR Method

Method	1D	2D	3D	4D
UPFRR	0.1136	0.3470	0.6676	1.0000
PFRR	0.1915	0.4281	0.7059	1.0000
PRR	0.7085	0.9902	1.0000	1.0000

- PRR shows that 1st 2 components account for 99.02% of variance  
 $\Rightarrow$  **UPFRR** and **PFRR** may overestimate the number of dimensions



# Real data analysis I (case 2: $p \geq n$ , $r < n$ )

## Trace correlation coefficients (Hooper, 1959)

Given two matrices  $A_1$  and  $A_2$ ,  $q$  is the number of principal components to consider:

$$\bar{r} = \sqrt{\frac{\sum_{i=1}^q \lambda_i}{q}}$$

where  $\lambda_i$  are the eigenvalues of the matrix  $P = A_1^T A_2 A_2^T A_1$ .

**Table 4.** Trace Correlation Coefficients for **UPFRR**, **PFRR**, and **PRR**

Comparison	1st 2 components	1st 3 components
UPFRR vs PFRR	0.9247	1.0000
UPFRR vs PRR	0.9218	1.0000
PFRR vs PRR	1.0000	1.0000

- Similarity in the 1st 2 components suggests 2-dimensional **Ry** is sufficient  
⇒ Apply **PFRR** to reduce **Y** ( $r = 4$ ) → **Ry** ( $r' = 2$ )



# Real data analysis I (case 2: $p \geq n$ , $r < n$ )

- In  $\mathbf{Ry}$  ( $r' = 2$ ),
  - 1st component: linear combination of sucrose (Y2), dry flour (Y3), water (Y4)
  - 2nd component: fat (Y1)

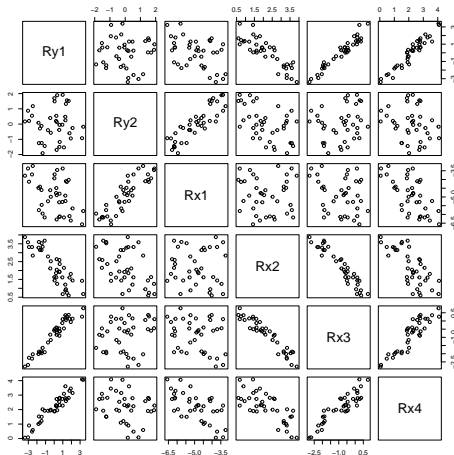


Figure 1. Scatter plot matrix of  $(\mathbf{Ry}, \mathbf{Rx})$  for cookie data





# Real data analysis I (case 2: $p \geq n$ , $r < n$ )

- **(Ry, Rx), (Y, Rx):** Analyze using **multivariate linear regression**
- **(Ry, X), (Y, X):** Analyze using **partial least squares regression**
  - `mvr` function from `pls` package (Liland et al., 2021)
- **Mean Squared Prediction Error (MSPE)**

$$\text{MSPE} = \frac{1}{n \times r} \sum_{i=1}^n \sum_{j=1}^r (y_{ij} - \hat{y}_{ij})^2$$

**Table 5. MSPE Results for cookie data**

Model	Y1	Y2	Y3	Y4
<b>(Ry, Rx)</b>	0.0901	0.0462	0.0452	0.0471
<b>(Y, Rx)</b>	0.0937	0.0463	0.0506	0.0470
<b>(Ry, X)</b>	0.0397	0.0418	0.0462	0.0400
<b>(Y, X)</b>	0.0396	0.0418	0.0495	0.0392

- Comparing **(Ry, Rx)** vs **(Y, Rx)** and **(Ry, X)** vs **(Y, X)**  
⇒ No substantial difference in prediction performance



# Real data analysis II (case 3: $p < n$ , $r \geq n$ )

## Nutrimouse data

- **nutrimouse** dataset from the **seedCCA** package (Kim et al., 2021)
  - $X_1$ : **genotypes** - wild type, PPARalpha
  - $X_2$ : **diets** - COC(coconut oil), FISH(fish oil), LIN(linseed oil), REF(corn and colza oil), SUN(sunflower oil)
  - $Y$  ( $r = 141$ ): 120 genes and 21 lipids
  - $n = 40$  ( $n < r$ )  $\Rightarrow$  **Require reducing  $r$**
  - Predictors are **categorical**, **PRR** is the preferable choice

**Table 6. Cumulative Variance** of 1-6 Dimensions with **PRR** Method for **nutrimouse** data

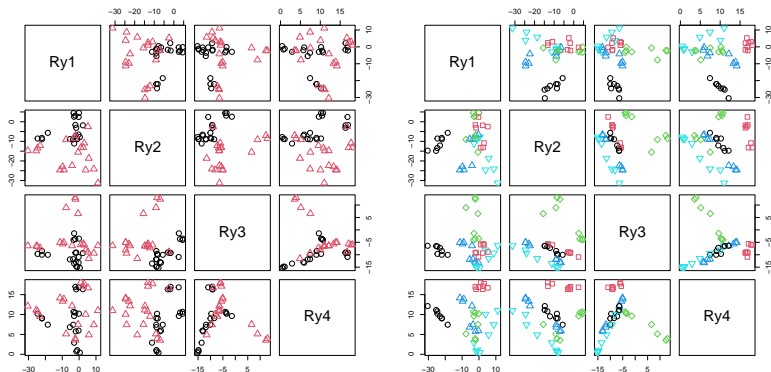
Dimension	1D	2D	3D	4D	5D	6D
Variance	0.4038	0.6949	0.8623	0.9554	0.9726	0.9835

- Based on **PRR**, 1st 4 components capture over 95% of total variance  
 $Y$  ( $r = 141$ )  $\rightarrow$   $Ry$  ( $r' = 4$ )



# Real data analysis II (case 3: $p < n$ , $r \geq n$ )

**Figure 2.** Scatter plot matrices of the reduced responses marked by **genotype** and **diet**



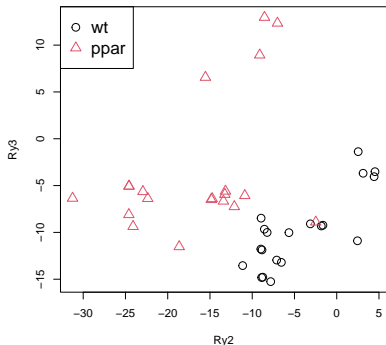
(a) Scatter plot matrix marked by **genotype** (b) Scatter plot matrix marked by **diet**

- **Ry2 & Ry3** distinctly separate **genotypes**, **Ry1 & Ry4** distinctly separate **diets**

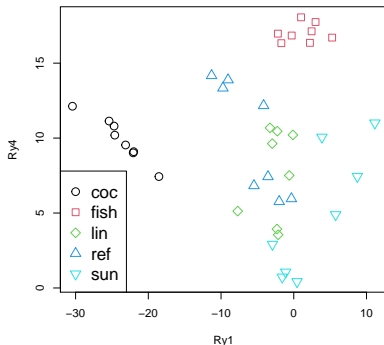


# Real data analysis II (case 3: $p < n$ , $r \geq n$ )

**Figure 3.** Scatter plots of **Ry2** and **Ry3** marked by genotype and of **Ry1** and **Ry4** marked by diet



(a) Plot of **Ry2** and **Ry3** (genotype)



(b) Plot of **Ry1** and **Ry4** (diet)

- **Ry2** & **Ry3** associated with **genotype**, **Ry1** & **Ry4** associated with **diet**  
⇒ possible existence of interaction between **genotype** and **diet**



# Real data analysis II (case 3: $p < n$ , $r \geq n$ )

**Table 7. MANOVA Results for `nutrimouse` data**

Effect	df	Pillai's trace	Approx. F	Pr(>F)
Genotype	1	0.9070	65.825	<b>1.574e-13 ***</b>
Diet	4	3.0805	25.125	<b>&lt; 2.2e-16 ***</b>
Genotype:Diet	4	2.0993	8.284	<b>4.339e-13 ***</b>
Residuals	30	-	-	-

- **MANOVA** with **Ry** shows that the effects of genotype, diet and their interaction are significant at 5%



# Real data analysis II (case 3: $p < n$ , $r \geq n$ )

- Split the data according to **genotype** (wild type, PPARAlpha)
- Compare dietary **factor-level means** using **test** function in **lsmeans** package (Lenth, 2016)

**Table 8.** Pairwise Comparison Results for **nutrimouse** data

Contrast	Estimate	df	t-ratio	p-value	Contrast	Estimate	df	t-ratio	p-value
coc-fish	-8.935	15	-23.833	<.0001	coc-fish	-9.817	15	-15.126	<.0001
coc-lin	-9.714	15	-25.912	<.0001	coc-lin	-9.370	15	-14.437	<.0001
coc-ref	-3.401	15	-9.072	<.0001	coc-ref	-2.794	15	-4.305	0.0008
coc-sun	-1.627	15	-4.341	0.0006	coc-sun	-4.435	15	-6.833	<.0001
fish-lin	-0.779	15	-2.079	0.0552	fish-lin	0.447	15	0.689	0.5013
fish-ref	5.534	15	14.762	<.0001	fish-ref	7.023	15	10.821	<.0001
fish-sun	7.308	15	19.492	<.0001	fish-sun	5.382	15	8.293	<.0001
lin-ref	6.313	15	16.841	<.0001	lin-ref	6.576	15	10.132	<.0001
lin-sun	8.087	15	21.571	<.0001	lin-sun	4.935	15	<.0001	<.0001
ref-sun	1.774	15	4.731	0.0003	ref-sun	-1.641	15	0.0258	0.0258

(a) Pairwise Comparison in **Wild Type**

(b) Pairwise Comparison in **PPARAlpha**

- In **Wild Type**, all diets are different from each other
- In **PPARAlpha**, **FISH** and **LIN** are not distinguishable



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# Summary and Limitations

## ● Summary

- Demonstrate the practical application of **Response Dimension Reduction** across different relationships between  $p, r, n$
- Apply to **cookie** data (**case 2**:  $n \leq p$ ), **nutrimouse** data (**case 3**:  $n \leq r$ )
  - Achieve simplified information while maintaining predictive performance

## ● Limitations

- Beyond **case 1**, it is hard to capture **nonlinear relationship**
- Absence of real data applications for **case 4**:  $n \leq \min(p, r)$
- Variable performance of RDR methods across different datasets





Thank You.



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