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of ACE

Applications
ACE v.s. NN

An Introduction to Alternating Conditional Expectation (ACE) Algorithm

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Correlation between random variables

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Pearson correlation coefficient

$$\rho(X, Y) \triangleq \frac{\mathbb{E}[XY] - \mathbb{E}[X] \mathbb{E}[Y]}{\sqrt{\text{Var}(X)} \sqrt{\text{Var}(Y)}}$$

- $|\rho(X, Y)| \leq 1$

HGR correlation

$$\rho_m(X, Y) \triangleq \max_{f, g} \rho(f(X), g(Y))$$

- $|\rho(X, Y)| \leq \rho_m(X, Y) \leq 1$



HGR correlation for discrete random variables

$$\rho_m(X, Y) \triangleq \max_{f, g} \rho(f(X), g(Y)) = \max_{\substack{f: \mathbb{E}[f]=0, \text{Var}(f)=1 \\ g: \mathbb{E}[g]=0, \text{Var}(g)=1}} \mathbb{E}[f(X)g(Y)]$$

Discrete (and finite) alphabet

X, Y take values from $\mathcal{X} = \{1, \dots, |\mathcal{X}|\}$ and $\mathcal{Y} = \{1, \dots, |\mathcal{Y}|\}$, respectively.

$$\begin{aligned} \mathbb{E}[f(X)g(Y)] &= \sum_{x \in \mathcal{X}, y \in \mathcal{Y}} P_{X,Y}(x, y) f(x) g(y) \\ &= \sum_{x=1}^{|\mathcal{X}|} \sum_{y=1}^{|\mathcal{Y}|} f(x) \sqrt{P_X(x)} \cdot \frac{P_{X,Y}(x, y)}{\sqrt{P_X(x)} \sqrt{P_Y(y)}} \cdot g(y) \sqrt{P_Y(y)} \end{aligned}$$



HGR correlation for discrete random variables

$$\rho_m(X, Y) \triangleq \max_{f, g} \rho(f(X), g(Y)) = \max_{\substack{f: \mathbb{E}[f]=0, \text{Var}(f)=1 \\ g: \mathbb{E}[g]=0, \text{Var}(g)=1}} \mathbb{E}[f(X)g(Y)]$$

Discrete (and finite) alphabet

X, Y take values from $\mathcal{X} = \{1, \dots, |\mathcal{X}|\}$ and $\mathcal{Y} = \{1, \dots, |\mathcal{Y}|\}$, respectively.

$$\begin{aligned} \mathbb{E}[f(X)g(Y)] &= \sum_{x \in \mathcal{X}, y \in \mathcal{Y}} P_{X,Y}(x, y) f(x) g(y) \\ &= \sum_{x=1}^{|\mathcal{X}|} \sum_{y=1}^{|\mathcal{Y}|} \underbrace{f(x) \sqrt{P_X(x)}}_{\phi(x)} \cdot \underbrace{\frac{P_{X,Y}(x, y)}{\sqrt{P_X(x)} \sqrt{P_Y(y)}}}_{B(y, x)} \cdot \underbrace{g(y) \sqrt{P_Y(y)}}_{\psi(y)} \end{aligned}$$



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HGR correlation for discrete random variables

Notations

- $\phi \leftrightarrow f : \phi(x) \triangleq \sqrt{P_X(x)}f(x)$
- $\psi \leftrightarrow g : \psi(y) \triangleq \sqrt{P_Y(y)}g(y)$
- $\mathbf{B} \leftrightarrow P_{X,Y} :$
$$B(y, x) \triangleq \frac{P_{Y,X}(y, x)}{\sqrt{P_Y(y)}\sqrt{P_X(x)}}$$

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- $\mathbf{B} \leftrightarrow P_{X,Y} :$

$$B(y, x) \triangleq \frac{P_{Y,X}(y, x)}{\sqrt{P_Y(y)}\sqrt{P_X(x)}}$$

$$\mathbb{E}[f] = \langle \phi, \mathbf{v}_0 \rangle, \quad v_0(x) = \sqrt{P_X(x)},$$

$$\mathbb{E}[g] = \langle \psi, \mathbf{u}_0 \rangle, \quad u_0(y) = \sqrt{P_Y(y)},$$

$$\mathbb{E}[f^2] = \|\phi\|^2, \quad \mathbb{E}[g^2] = \|\psi\|^2,$$

$$\mathbb{E}[f(X)g(Y)] = \psi^T \mathbf{B} \phi.$$

$$\mathbf{B} \phi \leftrightarrow \mathbb{E}[f(X)|Y], \quad \mathbf{B}^T \psi \leftrightarrow \mathbb{E}[g(Y)|X]$$

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HGR correlation for discrete random variables

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- $\mathbf{B} \leftrightarrow P_{X,Y} :$

$$B(y, x) \triangleq \frac{P_{Y,X}(y, x)}{\sqrt{P_Y(y)} \sqrt{P_X(x)}}$$

$$\mathbb{E}[f] = \langle \phi, \mathbf{v}_0 \rangle, \quad v_0(x) = \sqrt{P_X(x)},$$

$$\mathbb{E}[g] = \langle \psi, \mathbf{u}_0 \rangle, \quad u_0(y) = \sqrt{P_Y(y)},$$

$$\mathbb{E}[f^2] = \|\phi\|^2, \quad \mathbb{E}[g^2] = \|\psi\|^2,$$

$$\mathbb{E}[f(X)g(Y)] = \psi^T \mathbf{B} \phi.$$

$$\mathbf{B} \phi \leftrightarrow \mathbb{E}[f(X)|Y], \quad \mathbf{B}^T \psi \leftrightarrow \mathbb{E}[g(Y)|X]$$

$$\rho_m(X, Y) = \max_{\substack{f: \mathbb{E}[f]=0, \text{Var}(f)=1 \\ g: \mathbb{E}[g]=0, \text{Var}(g)=1}} \mathbb{E}[f(X)g(Y)] = \max_{\substack{\phi: \langle \phi, \mathbf{v}_0 \rangle=0, \|\phi\|=1 \\ \psi: \langle \psi, \mathbf{u}_0 \rangle=0, \|\psi\|=1}} \psi^T \mathbf{B} \phi$$



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Matrix B

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Definition

$$\mathbf{B} \leftrightarrow P_{X,Y} : \quad B(y, x) \triangleq \frac{P_{Y,X}(y, x)}{\sqrt{P_Y(y)}\sqrt{P_X(x)}}$$

Properties

- $\mathbf{u}_0 = \mathbf{B}\mathbf{v}_0, \mathbf{v}_0 = \mathbf{B}^T\mathbf{u}_0.$
- $\|\mathbf{B}\|_2 = 1.$
- The SVD of \mathbf{B} : $\mathbf{B} = \sum_{i=0}^K \sigma_i \mathbf{u}_i \mathbf{v}_i^T, \sigma_0 = 1 \geq \sigma_1 \geq \cdots \geq \sigma_K.$



Matrix B

Definition

$$\mathbf{B} \leftrightarrow P_{X,Y} : \quad B(y, x) \triangleq \frac{P_{Y,X}(y, x)}{\sqrt{P_Y(y)}\sqrt{P_X(x)}}$$

Properties

- The SVD of \mathbf{B} : $\mathbf{B} = \sum_{i=0}^K \sigma_i \mathbf{u}_i \mathbf{v}_i^T$, $\sigma_0 = 1 \geq \sigma_1 \geq \dots \geq \sigma_K$.
- $\sigma_1 = \max_{\substack{\phi: \langle \phi, \mathbf{v}_0 \rangle = 0, \|\phi\|=1 \\ \psi: \langle \psi, \mathbf{u}_0 \rangle = 0, \|\psi\|=1}} \psi^T \mathbf{B} \phi$, with $\phi^* = \mathbf{v}_1, \psi^* = \mathbf{u}_1$.



Matrix \tilde{B}

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Definition

$$\tilde{B} \triangleq B - u_0 v_0^T$$

$$\max_{\substack{\phi: \langle \phi, v_0 \rangle = 0, \|\phi\| = 1 \\ \psi: \langle \psi, u_0 \rangle = 0, \|\psi\| = 1}} \psi^T B \phi = \max_{\phi, \psi: \|\phi\| = \|\psi\| = 1} \psi^T \tilde{B} \phi$$



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Power method and ACE(Alternating Conditional Expectation)

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Power method

```
 $\phi \leftarrow \phi_0 ; \quad /* \text{ Initialization } */$   
 $\phi \leftarrow \phi - \langle \phi, v_0 \rangle v_0 ; \quad /* \phi \perp v_0 */$   
repeat  
     $\psi \leftarrow B\phi ;$   
     $\phi \leftarrow B^T \psi ;$   
     $\phi \leftarrow \phi / \|\phi\| ;$   
until  $\psi^T B \phi$  stops to increase;
```



Power method and ACE(Alternating Conditional Expectation)

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Power method

```
 $\phi \leftarrow \phi_0 ; \quad /* \text{ Initialization } */$   
 $\phi \leftarrow \phi - \langle \phi, v_0 \rangle v_0 ; \quad /* \phi \perp v_0 */$   
repeat  
     $\psi \leftarrow B\phi ;$   
     $\phi \leftarrow B^T \psi ;$   
     $\phi \leftarrow \phi / \|\phi\| ;$   
until  $\psi^T B \phi$  stops to increase;
```

ACE

```
 $g \leftarrow g_0 ; \quad /* \text{ Initialization } */$   
 $g(y) \leftarrow g(y) - \mathbb{E}[g(Y)] ; /* \text{ Center } */$   
repeat  
     $f(X) \leftarrow \mathbb{E}[g(Y)|X];$   
     $g(Y) \leftarrow \mathbb{E}[f(X)|Y];$   
     $g(Y) \leftarrow g(Y) / \sqrt{\mathbb{E}[g^2(Y)]};$   
until  $\mathbb{E}[f(X)g(Y)]$  stops to increase;
```




ACE for multiple modes

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Orthogonalization



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SVD & low rank approximation

Eckart-Young-Mirsky theorem

Suppose $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$, then $\mathbf{A}_r = \mathbf{U}_r\mathbf{\Sigma}_r\mathbf{V}_r^T$ is the optimal solution to the following low rank approximation problem:

$$\begin{aligned} & \underset{\hat{\mathbf{A}}}{\text{minimize}} && \|\mathbf{A} - \hat{\mathbf{A}}\|_F^2 \\ & \text{subject to} && \text{rank}(\hat{\mathbf{A}}) \leq r. \end{aligned}$$

Corollary

The solutions of

$$\underset{(\phi, \psi)}{\text{minimize}} \|\tilde{\mathbf{B}} - \psi\phi^T\|_F^2$$

are $\{(c\mathbf{v}_1, \frac{\sigma_1}{c}\mathbf{u}_1) : c \neq 0\}$.

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SVD & low rank approximation

Corollary

The solutions of

$$\underset{(\phi, \psi): \phi \perp \mathbf{v}_0, \psi \perp \mathbf{u}_0}{\text{minimize}} \quad \|\mathbf{B} - \psi\phi^T\|_F^2$$

are $\{(c\mathbf{v}_1, \frac{\sigma_1}{c}\mathbf{u}_1) : c \neq 0\}$.

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Corollary

The solutions of

$$\underset{(\phi, \psi): \phi \perp \mathbf{v}_0, \psi \perp \mathbf{u}_0}{\text{minimize}} \quad \|\mathbf{B} - \psi \phi^T\|_F^2$$

are $\{(c\mathbf{v}_1, \frac{\sigma_1}{c}\mathbf{u}_1) : c \neq 0\}$.

$$\frac{1}{2} \|\mathbf{B} - \psi \phi^T\|_F^2 = \frac{1}{2} \|\mathbf{B}\|_F^2 - \left[\psi^T \mathbf{B} \phi - \frac{1}{2} \cdot (\phi^T \phi) \cdot (\psi^T \psi) \right]$$

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SVD & low rank approximation

Corollary

The solutions of

$$\underset{(\phi, \psi): \phi \perp \mathbf{v}_0, \psi \perp \mathbf{u}_0}{\text{minimize}} \quad \|\mathbf{B} - \psi\phi^T\|_F^2$$

are $\{(c\mathbf{v}_1, \frac{\sigma_1}{c}\mathbf{u}_1) : c \neq 0\}$.

$$\frac{1}{2}\|\mathbf{B} - \psi\phi^T\|_F^2 = \frac{1}{2}\|\mathbf{B}\|_F^2 - \underbrace{\left[\psi^T \mathbf{B} \phi - \frac{1}{2} \cdot (\phi^T \phi) \cdot (\psi^T \psi) \right]}_{H(\phi, \psi)}$$



SVD & low rank approximation

Corollary

The solutions of

$$\underset{(\phi, \psi): \phi \perp \mathbf{v}_0, \psi \perp \mathbf{u}_0}{\text{minimize}} \quad \|\mathbf{B} - \psi\phi^T\|_F^2$$

are $\{(c\mathbf{v}_1, \frac{\sigma_1}{c}\mathbf{u}_1) : c \neq 0\}$.

$$\frac{1}{2}\|\mathbf{B} - \psi\phi^T\|_F^2 = \frac{1}{2}\|\mathbf{B}\|_F^2 - \underbrace{\left[\psi^T \mathbf{B} \phi - \frac{1}{2} \cdot (\phi^T \phi) \cdot (\psi^T \psi) \right]}_{H(\phi, \psi)}$$

$$H(f(X), g(Y)) \triangleq \mathbb{E}[f(X)g(Y)] - \frac{1}{2} \cdot \text{Var}(f(X)) \cdot \text{Var}(g(Y)).$$



H-score

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$$H(f(X), g(Y)) \triangleq \mathbb{E}[f(X)g(Y)] - \frac{1}{2} \cdot \text{Var}(f(X)) \cdot \text{Var}(g(Y)).$$

$$H(f(X)) \triangleq \max_g H(f(X), g(Y)) = \frac{1}{2} \cdot \frac{\text{Var}(\mathbb{E}[f(X)|Y])}{\text{Var}(\mathbb{E}[f(X)])}.$$



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The geometry of ACE

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Principal Angles



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Theoretical results

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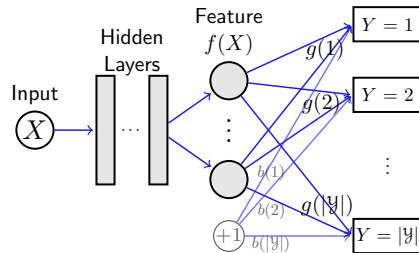
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H-score v.s. Log-loss

- Local assumption: X and Y are nearly independent.

- $\ell_{\log} \approx -\frac{1}{2}H(\mathbf{f}(X), \mathbf{g}(Y)) + C$



$$\tilde{P}_{Y|X}(y|x) \triangleq \frac{e^{f^T(x)g(y)+b(y)}}{\sum_{y' \in \mathcal{Y}} e^{f^T(x)g(y')+b(y')}}$$

Softmax Output



Applications

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NN for ACE

H-score & ACE-Net:

Warning

Outliers in ACE

Extensions

MACE: Modified(Multiple) ACE Algorithm



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- [1] Leo Breiman and Jerome H Friedman.
Estimating optimal transformations for multiple regression and correlation.
Journal of the American statistical Association, 80(391):580–598, 1985.
- [2] Hans Gebelein.
Das statistische problem der korrelation als variations-und eigenwertproblem und sein
zusammenhang mit der ausgleichsrechnung.
*ZAMM-Journal of Applied Mathematics and Mechanics/Zeitschrift für Angewandte Mathematik
und Mechanik*, 21(6):364–379, 1941.
- [3] Hermann O Hirschfeld.
A connection between correlation and contingency.
In *Mathematical Proceedings of the Cambridge Philosophical Society*, volume 31, pages 520–524.
Cambridge University Press, 1935.
- [4] Shao-Lun Huang, Anuran Makur, Lizhong Zheng, and Gregory W Wornell.
An information-theoretic approach to universal feature selection in high-dimensional inference.
In *Information Theory (ISIT), 2017 IEEE International Symposium on*, pages 1336–1340. IEEE,
2017.



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- [5] Shao-Lun Huang, Lin Zhang, and Lizhong Zheng.
An information-theoretic approach to unsupervised feature selection for high-dimensional data.
In *Information Theory Workshop (ITW), 2017 IEEE*, pages 434–438. IEEE, 2017.
- [6] Anuran Makur, Fabián Kozynski, Shao-Lun Huang, and Lizhong Zheng.
An efficient algorithm for information decomposition and extraction.
In *Communication, Control, and Computing (Allerton), 2015 53rd Annual Allerton Conference on*, pages 972–979. IEEE, 2015.
- [7] Alfréd Rényi.
On measures of dependence.
Acta mathematica hungarica, 10(3-4):441–451, 1959.



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Thank you!