# Statistical Learning Theory summary

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This summary has been written based on the Lecture 252-0526-00 S Statistical Learning Theory by Prof. J. M. Buhmann (Spring 2023). This serves as complementary summary to the lecture script which is also allowed to take to the exam. There is no guarantee for completeness and/or correctness regarding the content of this summary. Use it at your own discretion

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Generative model: 1. select x_i \in \mathcal{X}
                                                                                                                                                 \frac{\partial}{\partial \theta} \sum_{c} Rp(c|\ldots) = 0 \to \sum_{c} p(c|\ldots) (\frac{\partial}{\partial \theta} R) = 0
S(1) = 0, S(u) > S(v) \rightarrow u < v, continu-
                                                                        minze mutual info) \rightarrow Minze cost \rightarrow Get
                                                                                                                                                DA: stop splitting via CV, MDL, PA
                                                                                                                                                                                                                         with unif 1/n; 2. choose clust us-
ous, S(uv) = S(u) + S(v) if indip, S(u) =
                                                                        c^{opt} \to \text{Constr} \text{ on context MI} \to \text{Feat space}
                                                                                                                                                                                                                         ing clust membership c(i) of x_i; select
-c \log u, c const Entropy: H(P(x)) =
                                                                                                                                                 Markov Chains \sum_{c'} P(c,c') = 1
                                                                                                                                                                                                                         y_i \in \mathcal{Y} \text{ from } q(y_i|c(i)). \quad \hat{p}(x_i,y_i) =
                                                                        Rate dist theory: d: \mathcal{X} \times \mathcal{X} \to \mathbb{R}^+, w
H(X) = \mathbb{E}_{x \sim P}[S] = -\sum_{x} P(x) \log P(x)
                                                                        \mathbb{E}_{x,\hat{x}}[d(x,\hat{x})] = \sum_{x \in \mathcal{X}} \sum_{\hat{x} \in \hat{\mathcal{X}}} p(\hat{x}|x) p(x) d(x,\hat{x})
                                                                                                                                                 P(X_{t+1} = c'|X_t = c) = P(c,c'), Irre-
Cont: H can \leq 0 unif (0, 1/2), Discr:
                                                                                                                                                 ducible: can go from any stato to any
                                                                        Shannon/Kolmogorov: opt repr satisfies
0 < H < \log N, H = 0 \text{ iff } \exists x : p(x) = 0
                                                                                                                                                 state (finite steps), Periodic: if state i is
                                                                        R(D) = \min_{\{p(\hat{x}|x): \mathbb{E}_{x,\hat{x}}[d(x,\hat{x})] < D\}} I(x,\hat{x})
1, N = |\mathcal{X}|, H_N(p(x_1)...p(x_N)) =
                                                                                                                                                 visited after number of steps multiple of
                                                                        L(p(\hat{x}|x)) = I(x,\hat{x}) + \beta(\mathbb{E}_{x,\hat{x}}[d(x,\hat{x})] - D)
H_{N-1}(p(x_1)+p(x_2),..)
                                                                                                                                                 integer d > 1 (d = 1 aperiodic), Station-
                                                                        \frac{\delta L}{\delta p(\hat{x}|x)} = 0 \Rightarrow p(\hat{x}|x) = \frac{p(\hat{x})}{Z(x,\beta)} \exp(-\beta d(x,\hat{x}))
+(p(x_1)+p(x_2))H_2(\frac{p(x_1)}{p(x_1)+p(x_2)},\frac{p(x_2)}{p(x_1)+p(x_2)})
                                                                                                                                                                                                                         P(x_i, y_i | c, q) = q(y_i | c(i)) p(c(i)), p(\alpha) = 1/k
                                                                                                                                                 arity: \sum_{c \in \mathcal{C}} \pi(c) P(c, c') = \pi(c'). If all
                                                                        Max Entropy: p(c|X) \propto \exp(-\beta R(c,X))
                                                                                                                                                 above satisfied, \lim_{t\to\infty} \mathbb{P}[X_t=c] = \pi(c),
BinH: H_{bin}(\delta) = -\delta \log \delta - (1-\delta) \log (1-\delta)
                                                                        Requirements for p(\cdot|X): R(c_1,X) \leq
ConH H(Y|X) = \int P(X=x)H(Y|X=x)
                                                                                                                                                 \lim_{t\to\infty}\frac{1}{t}\sum_{1}^{t}f(X_s) = \sum_{c}\pi(c)f(c), De-
)dx = \int p(x) \int p_{Y|X}(y,x) \log p_{Y|X}(y,x) dy dx \ R(c_2,X) \rightarrow p(c_1|X) \ge p(c_2|X), \ \text{Jaynes's}
                                                                                                                                                tailed balnc \pi(c)P(c,c') = \pi(c')P(c',c)
                                                                        (see below) p_{\beta}(c) = \exp[-\beta \cdot (R(c) - F(\beta))],
                                                                                                                                                Mixing time of MC \propto \frac{1}{\lambda_1 - \lambda_2} where \lambda_1 = 1
H(X,Y) = H(X) + H(Y|X) \text{ (CR)}
                                                                        Free energy F(\beta) = \mathbb{E}[R(c,X)] - T \cdot H =
                                                                                                                                                                                                                         \hat{p}(j|i)\log(\frac{\hat{p}(j|i)}{q(j|c(i))}) - l\sum_{i}\hat{p}(i)\log p(c(i))
MI I(X;Y) = I(Y;X) = H(X) - H(X|Y)
                                                                                                                                                 is first eig and \lambda_2 \leq \lambda_1 is second eig of P.
                                                                        -\frac{1}{\beta}\log Z(\beta). Gibbs free energy: G(p)=
= \mathbb{E}_{X,Y}[\log \frac{p(X,Y)}{p(X)p(Y)}], I(X;X) = H(X)
                                                                                                                                                 Least Angle Clustering e_i := X_i/|X_i|
                                                                        \sum_{c \in C} p(c)R(c) + \frac{1}{\beta} \sum_{c} p(c) \log p(c),
ConI I(X;Y|Z) = H(X|Z) - H(X|Y,Z)
                                                                                                                                                 S(x_i, x_j) = w_{ij} \cos \phi_{ij} = w_{ij} e_i e_j, w_{ij} = v_i \cdot v_j
                                                                        G(p) = \frac{1}{\beta} KL(p||p_{\beta}) + F(\beta)
I(X,Y;Z) = H(X,Y) - H(X,Y|Z) =
                                                                                                                                                 v_i = 1/\sqrt{p_k n}, p_k = \frac{1}{n} \sum_i M_{ik}, v_i v_j = \frac{1}{n_i n_i} = \bullet
H(X) + H(Y|X) - H(X|Z) - H(Y|X,Z) =
                                                                        Measurements: r_i(x), 1 \leq j \leq m, yield
                                                                                                                                                 R(M,X) = \frac{1}{2} \sum_{\nu}^{k} \sum_{i}^{n} \sum_{j}^{n} M_{i\nu} M_{j\nu} v_{i} v_{j} \cos \phi_{ij}
I(X;Z) + I(Y;Z|X) Given X
                                                                        constraints \mathbb{E}\{r_j(X)\} = \mu_j. Jaynes's
                                                                                                                                                                                                                         \frac{\partial}{\partial q_{ja}} \sum_{\nu} \lambda_{\nu} \sum_{j} (q_{jv} - 1), p_{i}(\alpha | Q, \mathcal{X})
Y \rightarrow Z: I(X;Z) \leq I(X;Y) Chain:
                                                                        principle \sup_{p(X)} \{-\int_{\mathcal{X}} p(x) \log p(x) dx\},
                                                                                                                                                +\frac{1}{2}\sum_{\nu}^{k}\sum_{i}^{n}M_{i\nu}^{2}v_{i}^{2}=k/2
I(X;Y,Z) = I(X;Y) + I(X;Z|Y) =
                                                                                                                                                                                                                         Limitations: lack topology (permutations
                                                                         \int_{\mathcal{V}} p(x)dx = 1 p(x) \ge 0, \int_{\mathcal{V}} p(x)r_i(x)dx = 0
                                                                                                                                                Z = \sum_{\{M\}} \prod_{\nu=1}^{k} \exp(\frac{\beta p_{\nu} n}{2} \| \frac{1}{p_{\nu} n} \sum_{i=1}^{n} M_{i\nu} e_i \|^2
I(X;Z) + I(X;Y|Z).
                                                                        \mu_j, 1 \leq j \leq m \ J(p + \delta p) = \int_x (p + \delta p)
                                                                                                                                                 y_{\alpha} = \frac{1}{n_{\alpha}n} \sum_{i=1}^{n} e_{i} p_{i\alpha}, p_{\alpha} = \frac{1}{n} \sum_{i=1}^{n} p_{i\alpha}
I(X_1, ... X_n; Z) = \sum_{i=1}^{n} I(X_i; Z | X_1, ... X_{i-1})
                                                                         (-\log(p(1+\delta p/p)) + \lambda_0 - \sum_{j=1}^m \lambda_j r_j(x)) dx.
DPi: I(X;Y|Z) \ge 0 and I(X;Z|Y) = 0
                                                                                                                                                Laplace: f(x^*) = 0, I = \int d\mathbf{x} h(\mathbf{x}) e^{-nf(\mathbf{x})}
                                                                        Variation equal zero:
X_1 \to ... \to X_n, I(X_1; X_2..X_n) = I(X_1; X_2)
                                                                                                                                                 f(\mathbf{x}) \approx f(x^*) + \frac{1}{2}(x - x^*)^{\top} H_f(x^*)(x - x^*)
                                                                         \frac{1}{Z}\exp(-\sum_{1}^{m}\lambda_{j}r_{j}(x)), \quad Z = \int_{x}\dots \mathbf{TTL}
KL D_{KL}(p||q) = \sum_{x} p(x) \log(\frac{p(x)}{q(x)})
                                                                                                                                                I \approx e^{-nf(x^*)} \int h(x^*) e^{-\frac{n}{2}(x-x^*)^{\top} H_f(x^*)(x-x^*)}
                                                                        284: 0 = \int_x \frac{\partial p(x)}{\partial \mu_i} dx, 1 = \int_x \frac{\partial p(x)}{\partial \mu_i} r_i(x) dx
\mathbf{Msc}\ I(X;Y) = KL(p_{X,Y}(x,y)||p_X(x)p_Y(y))
                                                                                                                                                                                                                         by themselves).
                                                                                                                                                 H = Q^{\top} \Lambda Q, H^{1/2} = Q \Lambda^{1/2}, y = \sqrt{n} H^{1/2}(x - y)
H(X|Y) < H(X), H(X,Y|Z) > H(X|Z),
                                                                        1 \le \sqrt{\mathbb{E}[(\frac{\partial \log p(x)}{\partial \mu_i})^2]} \sqrt{\text{Var}[r_i(x)]}, \text{ estimated}
                                                                                                                                                (x^*), x = y \frac{H^{-1/2}}{\sqrt{n}} + x^* Jacobian, n^{-d/2} \det(\Lambda)^{1/2}
H(5X) = H(X) if X discrete, > H(X)
                                                                       error \mu_i \sim \sqrt{\operatorname{Var}\{r_i\}} \Rightarrow \delta\mu_i = \beta_i \sqrt{\operatorname{Var}\{r_i\}}
                                                                                                                                                I \approx e^{-nf(x^*)}h(x^*) \int dy \, e^{-\frac{\|y\|^2}{2}} \cdot |\det |J_y| = 0
cont. H(X,Y,Z) - H(X,Y) \le H(X,Z)
H(X), H(X|Y) \ge H(X|Y,Z), H(X,Y) \le
                                                                        \beta_i \le \sqrt{\mathbb{E}\left[\left(\frac{\delta_{\mu_i} p(x)}{p}\right)^2\right]}, \text{ eq. if } \frac{\partial \ln p(x)}{\partial \mu_i} \sim r_i(x) - \mu_i
                                                                                                                                                =rac{e^{-nf(x^*)}h(x^*)\cdot(2\pi)^{d/2}}{n^{d/2}\sqrt{\det(H_f(x^*))}} Gibbs distribution
H(X) + H(Y), H(g(X)) \leq H(X), X \text{ discr.}
                                                                        Distrib with min sensitivity: \frac{\partial \ln p(x)}{\partial \mu_i}
I(X,Y;Z) \geq I(X;Z), I(X;Z|Y)
                                                                                                                                                p(M|X) = \frac{1}{z} \exp(\frac{\beta}{2n} \sum_{\nu=1}^{k} \frac{1}{p_{\nu}} (\sum_{i=1}^{n} M_{i\nu} e_i)^2)
-I(Z;Y)+I(Z;Y|X)+I(X;Z),I(g(X),Y)
                                                                        \alpha_i(r_i(x) - \mu_i), \ \alpha_i \ \text{constants.} Cov matrix
                                                                                                                                                BW: e^{b^2/2a^2} = \int_{\mathbb{R}} \frac{a}{\sqrt{2\pi}} \exp(-\frac{a^2x^2}{2} + bx) dx
                                                                        C_{i,j} = \mathbb{E}(r_i(x) - \mu_i)(r_j(x) - \mu_j) is diag,
< I(X;Y) Codes: source code C for RV
X is map \mathcal{X} \to D^*, domain X, set of finite
                                                                        \alpha_i(\mu_1,\ldots,\mu_m) dep only on \mu_i \to \text{Gibbs}
                                                                                                                                                 Nominator: \sqrt{\beta n/\pi}^{dk} \prod_{\nu}^{k} p_{\nu}^{\frac{a}{2}} \int_{\mathbb{R}^{d}} dy_{1} \cdots dy_{k}
length strings from D-ary alphabeth.
                                                                        distr \rightarrow min sensitiv to change moments \mu_i.
                                                                                                                                                \exp(-\beta n(\frac{1}{2}\sum_{\nu}p_{\nu}y_{\nu}^{2}-\frac{1}{n}\sum_{\nu}y_{\nu}\sum_{i}M_{i\nu}e_{i}))
Exp length: L(C) = \sum_{x \in \mathcal{X}} P(x)l(x)
                                                                        Kmeans: R^{\text{km}}(c, \mathbf{Y}, \mathbf{X}) = \sum_{i \le n} ||x_i - y_{c(i)}||^2
Prefix code: no codeword is prefix of
                                                                                                                                                p_{\alpha}^* y_{\alpha}^* = \frac{1}{n} \sum_{i=1}^n e_i p_{i\alpha}^*, \ p_{i\alpha}^* = \frac{\exp(\beta e_i y_{\alpha}^*)}{\sum_{\nu=1}^k \exp(\beta e_i y_{\nu}^*)}
                                                                         \frac{\partial}{\partial y_{\alpha}} R^{\text{km}}(\ldots) = -2 \sum_{i:c(i)=\alpha} (x_i - y_{\alpha}) = 0
other cw. Kraft ineq: prefix code over
                                                                        y_{\alpha} = \frac{1}{n_{\alpha}} \sum_{i:c(i)=\alpha} x_i \text{ w} \setminus n_{\alpha} = \#\{i:c(i)=\alpha\}
                                                                                                                                                 Z = \int dy_1 ... \int dy_k \exp(-\beta n f_X(y)), p(M|X) \approx
|alphabet| = D: \sum_{i=1}^{m} D^{-l_i} \leq 1(l_i)
                                                                        Centroid equation: posterior p(c|X,\theta)
                                                                                                                                                        \exp(-\beta n(\frac{1}{2}\sum_{i}p_{\nu}^{*}y_{\nu}^{*^{2}}-\frac{1}{n}\sum_{\nu}y_{\nu}^{*}\sum_{i}M_{i\nu}e_{i}))
length code word)
                                                                                                                                                 \frac{1}{\exp(-\beta n(\frac{1}{2}\sum_{\nu}^{*}p_{\nu}^{*}y_{\nu}^{*}-\frac{1}{\beta n}\sum_{i=1}^{n}\log\sum_{\nu=1}^{n}\exp(\beta e_{i}y_{\nu}^{*})))}
                                                                        depends on \theta. ME for \theta, S = \text{entropy}:
Opt. codes: minimize L = \sum_{i=1}^{m} p_i l_i s.t.
                                                                        \frac{\partial}{\partial \theta} S = -\sum_{c} \left( \frac{\partial}{\partial \theta} p(c \mid x, \theta) \right) \log p(c \mid x, \theta) +
                                                                                                                                                 \exp(\beta \sum_{\nu} y_{\nu}^* \sum_{i} M_{i\nu} e_{i} - \sum_{i}^{n} \log \sum_{\nu}^{n} \exp(\beta e_{i} y_{\nu}^*))
\sum_{i=1}^{m} D^{-l_i} \leqslant 1 \Rightarrow L^{\star} = -\sum_{i=1}^{m} p_i \log p_i
Inform. Bottle: efficient code X \mapsto C
                                                                                                                                                 MAP: \frac{1}{n}\sum_{i}M_{i\alpha}e_{i}=\frac{1}{n}\sum_{i=1}^{n}e_{i}p_{i\alpha}^{*}
                                                                        \sum_{c} p(c|x,\theta) \frac{\frac{\partial}{\partial \theta} p(c|x,\theta)}{p(c|x,\theta)} = \beta \sum_{c} R(\frac{\partial}{\partial \theta} p(c \mid x,\theta))
                                                                                                                                                                                                                         n_{ij} = \# observation at site i is in I_i, \mathcal{L} =
```

Preserve relevant info on context variable

**Scheme:** Obj space → Data groups (by

 $Y \mathcal{R}^{IB} = I(X; C) - \lambda I(C; Y), \lambda > 0$ 

**Information Theory** 

Surprise:  $S(\mathbb{P}(A)) : [0,1] \rightarrow [0,\infty).$ 

 $\frac{1}{l} \sum_{r=1}^{l} \Delta_{x_i, x_{i(r)}} \Delta_{y_j, y_{j(r)}}, \quad \hat{p}(y_j | x_i)$  $\hat{p}(x_i,y_i)$  $\frac{\hat{p}(x_i)}{\hat{p}(x_i)} = \frac{1}{\frac{1}{l} \sum_{r=1}^{l} \sum_{j=1}^{m} \Delta_{x_i, x_i(r)} \Delta_{y_j, y_{j(r)}}}$  $\mathcal{L} = \prod_{i=1}^{n} \prod_{j=1}^{m} \mathbf{P}(x_i, y_j | c(i), q)^{l\hat{p}(x_i, y_j)}$ 

**Histo Cluster**  $\Delta_{i,j} = 1(0)$  **if**  $i = j (i \neq j)$ 

*n* obj, *m* feat, *l* dyads  $\{(x_{i(r)}, y_{j(r)})\}_{r=1}^{l}$ 

 $R^{\text{hc}}(c; \{q(\cdot|\alpha)\}) = -\log(\mathcal{L}), x_i \to i, y_j \to j$  $R^{\text{hc}} \to R^{\text{hc}} + l \sum_{i} \sum_{j} \hat{p}(j|i)\hat{p}(i) \log \hat{p}(j|i) =$  $\sum_{i} \hat{p}(i) \sum_{m} \hat{p}(j|i) (\log \hat{p}(j|i) - \log q(j|c(i)))$  $l\sum_{i}\sum_{j}\widehat{p(j|i)}\widehat{p(i)}\log(p(c(i))) = l\sum_{i}\widehat{p(i)}\sum_{j}$ 

 $\frac{\partial}{\partial \theta} \beta \sum_{c} Rp(c \mid x, \theta) = \frac{\partial}{\partial \theta} \mu = 0, \ \mu \text{ is guar-}$ 

anteed by Lagr variabl  $\beta$  (not dep on  $\theta$ )

 $\hat{p}(i) \approx 1/n$  since obj dawn from unif distrib  $R^{hc}(c,q,\hat{p}) \propto -l \sum_{i=1}^{n} \sum_{j=1}^{m} \hat{p}(i,j) \log q(j|c(i))$ Centr. cond:  $\mathbb{E}_{c|\hat{p}} \frac{\partial}{\partial a(i|\alpha)} R^{hc}(c,q,\hat{p}) = 0 =$  $-\sum_{i}\sum_{j}l\hat{p}(i,j)\mathbb{E}_{c|\hat{p}}\mathbb{I}_{\{c(i)=\alpha\}}\frac{\partial}{\partial q_{i\alpha}}\log q_{j\alpha}$  +

bin index do not change KL, neglect info due to noise-induced errors during the histogramming process ca), Histograms repr

cat info while most feat spaces equipped w\ natural topo (feature similarity), cant impose structure (idk nothing about pixels

PDC: replace empirical histogram centroids by prototypical distribution parametrized by Gaussian mixture (more robust centroids), assume given set of

obj  $\mathbf{o}_{i}, i \in \{1..n\}, M_{i\nu} = 1$ , if obj  $\mathbf{o}_{i}$  assigned to cluster  $\nu = 1..k$ ,  $\sum_{\nu \le k} M_{i\nu} = 1$ . Each obj  $\mathbf{o}_i$  equipped with set of  $n_i$ obs  $\mathcal{X}_i = \{x_{i1}, \dots, x_{in_i}\}, x_{ij} \in \mathbb{R}^d,$ 

 $p(x|\nu) = \sum_{\alpha=1}^{l} p_{\alpha|\nu} g(x|\mu_{\alpha}, \Sigma_{\alpha}), \text{ prob of }$ 

various groups  $p_{\nu}$ , feat val restr to specific domains → rectified Gauss. Domain  $I = \bigcup_{i=1}^m I_j, I_j \cap I_s = \emptyset$  for  $j \neq s$ , region weight  $G_a(j) = \int_{I_a} g_a(y) dy$ ,

 $\Theta = \{ p_{\nu}, p_{\alpha|\nu}, \mu_{\alpha} | \alpha = 1, \dots, l; \nu = 1, \dots k \}$ 

 $\mathcal{L} = \prod_{i \le n} \sum_{\nu \le k} M_{i\nu} p_{\nu} p(\mathcal{X}_i | \nu, \Theta) =$  $\prod_{i \leq n} \prod_{\nu \leq k} [p_{\nu} p(\mathcal{X}_i | \nu, \Theta)]^{M_{i\nu}}$ 

 $\prod_{i \le n} \prod_{\nu \le k} [p_{\nu} \prod_{j \le m} (\sum_{\alpha \le l} p_{\alpha|\nu} G_{\alpha}(j))^{n_{ij}}]^{M_{i\nu}}$ 

 $\mathcal{R}^{phc}(c, \{p(a|\nu)\}, \theta) = -\log \mathcal{L}, \text{ two-part}$ 

coding scheme: expected codelength when

encoding the cluster memberships and en-

coding the individual feat values.  $E[\mathcal{R}] =$ 

 $\sum_{i} \sum_{\nu} q_{i\nu} [\log p_{\nu} + \sum_{j} n_{ij} \log(\sum_{\alpha} p_{\alpha|\nu} \tilde{G}_{\alpha}(j))]$ 

**EM:** E-step:  $h_{i\nu} = -\log p_{\nu} - \sum_{j} n_{ij} \log($ 

 $\sum_{\alpha} p_{\alpha|\nu} G_{\alpha}(j), q_{i\nu} = \mathbb{E}[M_{i\nu}] = p(M_{i\nu})$ 

1)  $\propto \exp(-\frac{h_{i\nu}}{T})$ , M-step:  $p_{\nu} = \frac{1}{n} \sum_{i} q_{i\nu}$ 

X prob of choose obj i, assume  $p_i = 1/n$ 

 $\left(p\left(\nu|i\right) = M_{i\nu}\right) \quad \left(p\left(j|\nu\right) = \sum_{\alpha=1}^{L} p_{\alpha|\nu} G_{\alpha}\left(j\right)\right)$ 

 $r_{kk'}^{(\ell+1)} \ = \ \frac{\sum_{i,j \leq N} \mathbf{P}^*(M_{ik}M_{jk'} = 1 | r^{(\ell)}) S_{ij}}{\sum_{i,j < N} \mathbf{P}^*(M_{ik}M_{jk'} = 1 | r^{(\ell)})} \ \ \mathrm{cant}$ use, norm const of  $(\star)$  is  $\Theta(2^{N\times K})$  MFA:  $(\star) \approx \mathbf{q}(\cdot|r) = \arg\min_{a} D_{KL} (q \| \mathbf{P}^*(\cdot \mid r))$ with  $\mathbf{q}(M|r) = \prod_{i \le N, k \le K} \mathbf{q}_{ik}(M_{ik} \mid r),$  $\mathbf{q}_{ik}(M_{ik}|r) \text{ Ber, } \mathbf{P}^*(M_{ik}M_{ik'}=1|r) =$  $\mathbf{q}(M_{ik} = 1|r)\mathbf{q}(M_{ik'} = 1|r)$ Compute M from  $\mathbf{q}(\cdot \mid r)$ . return M, r. Graph partitioning,  $D_{ij} \in \mathbb{R}$ :  $\mathcal{R}^{gp}(c; \mathcal{D}) = \sum_{\nu \leq k} \sum_{(i,j) \in \mathcal{E}_{\nu\nu}} D_{ij} =$  $\sum_{(i,j)\in\mathcal{E}} D_{ij} - \sum_{\nu,\mu:\nu<\mu} \sum_{(i,j)\in\mathcal{E}_{\nu\mu}} D_{ij} =$ const  $-\sum_{\nu \leq k} \operatorname{cut}(\mathcal{G}_{\nu}(\mathcal{D}), \mathcal{V} \setminus \mathcal{G}_{\nu}(\mathcal{D})) =$  $\operatorname{const}_2 + \sum_{\nu \leq k} \operatorname{cut}(\mathcal{G}_{\nu}(\mathcal{S}), \mathcal{V} \setminus \mathcal{G}_{\nu}(\mathcal{S})).$  Problem: strong bias for unbalances (very small or large) clusters due to lack normalization. Alternative costs: Norm cut  $\mathcal{R}^{nc}(c;\mathcal{S}) =$  $\sum_{\nu \leq k} \left( \frac{\operatorname{cut}(\mathcal{G}_{\nu}, \mathcal{V} \setminus \mathcal{G}_{\nu})}{\operatorname{assoc}(\mathcal{G}_{\nu}, \mathcal{V})} \right) = k - \sum_{\nu \leq k} \left( \frac{\operatorname{assoc}(\mathcal{G}_{\nu}, \mathcal{G}_{\nu})}{\operatorname{assoc}(\mathcal{G}_{\nu}, \mathcal{V})} \right)$ Average cut  $\mathcal{R}^{\mathrm{ac}}(c;\mathcal{S}) = \sum_{\nu \leq k} (\frac{\mathrm{cut}(\mathcal{G}_{\nu}, \mathcal{V} \setminus \mathcal{G}_{\nu})}{|\mathcal{G}_{\nu}|})$ Min-Max  $\mathcal{R}^{\mathrm{mmc}}(c;\mathcal{S}) = \sum_{\nu \leq k} \left( \frac{\mathrm{cut}(\mathcal{G}_{\nu}, \mathcal{V} \setminus \mathcal{G}_{\nu})}{\mathrm{assoc}(\mathcal{G}_{\nu}, \mathcal{G}_{\nu})} \right)$ (biased over equipatitions), ARC:  $\mathcal{R}^{\text{rc}}(c; \mathcal{S}) =$  $\sum_{\mu=\nu+1}^{k} \operatorname{cut}(\mathcal{G}_{\nu}, \mathcal{G}_{\mu}) (|\mathcal{G}_{\nu}|^{-\frac{1}{p-1}} + |\mathcal{G}_{\mu}|^{-\frac{1}{p-1}})^{p-1}$ (p = 2 standard Ratio Cut, p = 1 multiway)Cheeger Cut), Chg. Cut  $\mathcal{R}^{\text{Cheeger}}(c;\mathcal{S}) =$ 

 $\mathbf{P}^{\star}(S, M|r) \propto \exp(-R(M, r)/T)$ , compute

now values for r that maximize  $H[\mathbf{P}^*(\cdot|r)]$ 

 $\arg\max_r H[\mathbf{P}^*(\cdot|r)] = \arg\max_r F[R(\cdot,r)]$ 

EM to compute  $(\star) = \arg \max \log \tilde{\mathbf{P}}(S|r)$ 

 $\sum_{M} \int_{S} \mathbf{P}(S, M|r) dS = \sum_{M} \prod_{i,j} \int_{S_{i,j}} \prod_{k,k'}$ 

 $\exp(-M_{ik}M_{jk'}(S_{ij} - r_{kk'})^2/T)dS_{ij}$  EM:

E-step compute  $\tilde{\mathbf{P}}(\cdot \mid S, r_0) = \mathbf{P}^*(\cdot \mid r)$ ,

M-step compute  $r^* = \arg\max_r Q(r, r_0)$ , w/

w/  $F[R(\cdot, r)] = \log(\sum_{M} \exp(-\frac{R(M, r)}{T}))$ 

w/  $\tilde{\mathbf{P}}(S \mid r)$  is the marginal pdf of  $(\star)$ 

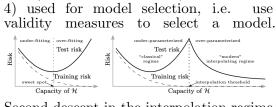
 $\operatorname{assoc}(A,V) - \operatorname{assoc}(A,A)$   $\perp$   $\operatorname{assoc}(B,V) - \operatorname{assoc}(B,B)$  $\operatorname{assoc}(A,V)$  $=2-\left(\frac{\operatorname{assoc}(A,A)}{\operatorname{assoc}(A,V)}+\frac{\operatorname{assoc}(B,B)}{\operatorname{assoc}(B,V)}\right)$ Constant Shift Embedding 12: end while  $\tilde{D}$  decomposition same D but tilde,  $\tilde{S}^c =$  $-\frac{1}{2}\tilde{D}^c, X_t = V_t(\Lambda_t)^{1/2}, Prob:$  cluster new obj given  $M \times N$  dissimilarities  $D_{ij}^{\text{new}}$  betw new obj and all n original Note:  $\tilde{S}^c V_p = V_p \Lambda_p \rightarrow X_p = \tilde{S}^c V_p (\Lambda_p)^{-1/2}$  $D^{new} \quad \frac{\text{Decomposition}}{D^{new}_{ij} = S^{new}_{ii} + \bar{S}^c_{ij} - 2S^{new}_{ij}} \\ S^{new} \quad \frac{Centralization}{(S^{new})^{c} - \frac{1}{n}[D^{new}([n - \frac{1}{n}O_n) - \frac{1}{n}e_ne_n^2] + \bar{D}([n - \frac{1}{n}e_ne_n^2])}}{(S^{new})^{c} - \frac{1}{n}e_ne_n^2]}$ truth/teacher information) or internal. MFA:  $c(i), c(j), i \neq j$  not dependent  $\frac{\partial^2 \mathcal{B}}{\partial q_u(\alpha) \partial q_v(\gamma)} = \frac{\partial h_u(\alpha)}{\partial q_v(\gamma)} = \sum_{c} \prod_{\substack{i=1 \ i \neq u, v}}^n q_i(c(i))$  $\mathbb{I}_{\{c(u)=\alpha,\,c(v)=\gamma\}}R(c,X)$ **MDS:** given **D**,  $\mathcal{Z} = \{\mathbf{z}_1, \dots, \mathbf{z}_n\} \subset \mathbb{R}^d$ find  $\mathbf{X} = {\mathbf{x}_1, \dots, \mathbf{x}_n} \subset \mathbb{R}^m, m = 1, 2, 3$  $J^{\operatorname{Sam} SStr}(\mathbf{X}, \mathbf{D}) = \sum_{i \leq n} \sum_{k \leq n} w_{ik} (\|\mathbf{x}_i - \mathbf{x}_i\|_{\mathbf{X}_i})$  $\|\mathbf{x}_k\|^2 - D_{ik}^2)^2 = \sum_{i,k \le n} w_{ik} (\|\mathbf{x}_i\|^2 + \|\mathbf{x}_k\|^2 - C_{ik}^2)^2$  $(2\mathbf{x}_{i}^{\top}\mathbf{x}_{k} + D_{ik}^{2}))^{2} = \sum_{i,k \leq n} w_{ik}(2\|\mathbf{x}_{i}\|^{4} +$  $2\|\mathbf{x}_i\|^2\|\mathbf{x}_k\|^2 - 8\|\mathbf{x}_i\|^2\mathbf{x}_i^{\top}\mathbf{x}_k - 4\|\mathbf{x}_i\|^2D_{i}^2 +$  $4\operatorname{Tr}(\mathbf{x}_i\mathbf{x}_i^{\top})(\mathbf{x}_k\mathbf{x}_k^{\top}) + 4\mathbf{x}_i^{\top}\mathbf{x}_kD_{ik}^2 + D_{ik}^4),$ SSTRESS (quartic cost func)  $\rightarrow$  analysed w\ linear algebra, SAMMONs (irrational cost func) mapping smoother embeddings  $k' \to \#$  param in model enc. by MLE  $\Theta_k$ than SSTRESS. Metric MDS:  $D(\cdot)$  yields **BIC:** dim  $\theta = p$ ,  $f'(x)_{x=x_0} = 0$ , flat prior numerical values meaningful/interpretable.  $p(M|X) = \frac{p(M)}{p(X)} \int \exp(\log p(X|M,\theta)) p(\theta|M) d\theta$ Non-Metric MDS:  $D(\cdot)$  respects rank dissimilarities, but not necessarily their numer- $\int_{\mathbb{R}} \exp(cf(x)) dx \propto \sqrt{2\pi} C|f''(x_0)| \exp(cf(x_0))$ ical values,  $\delta_{ij} < \delta_{kl} \to D(\delta_{ij}) < D(\delta_{kl})$ .  $0 = \frac{\partial \mathcal{D}^{\mathrm{KL}}(\mathbf{P}^0 \| \mathbf{P}^G)}{\beta \partial \theta_{ip}} = \alpha_i^0 \frac{\partial \mathbb{E}\{\|\mathbf{x}_i\|^4\}}{\partial \theta_{ip}} +$  $\sum_{\nu=1}^{k} \sum_{\mu=\nu+1}^{k} \left( \frac{\operatorname{cut}(\mathcal{G}_{\nu}, \mathcal{G}_{\mu})}{\min\{|\mathcal{G}_{\nu}|, |\mathcal{G}_{\mu}|\}} \right). \quad \mathbf{Validation} \quad + \hat{\mathbf{h}}_{i}^{T} \frac{\partial \mathbb{E}\{\|\mathbf{x}_{i}\|^{2} \mathbf{x}_{i}\}}{\partial \theta_{ip}} + \frac{\partial}{\partial \theta_{ip}} \operatorname{Tr}[\mathbf{H}_{i} \mathbb{E}\{\mathbf{x}_{i} \mathbf{x}_{i}^{T}\}] + \frac{\partial}{\partial \theta_{ip}} \operatorname{Tr}[\mathbf{H}_{i} \mathbb{E}\{\mathbf{x}_{i}^{T}\}] +$ 

of graph based methods poor understood

and no general accepted principle available.

Data space: pow(2,  $\binom{n}{2}$ )), Sol spc:  $2^n$ .  $\mathbf{h}_{i} = 8 \sum_{k=1}^{N} w_{ik} (D_{ik}^{2} \mathbb{E} \{ \mathbf{x}_{k} \} - \mathbb{E} \{ \| \mathbf{x}_{k} \|^{2} \mathbf{x}_{k} \} ),$ Data space is exponentially larger than  $\mathbf{H}_{i} = \sum_{k=1}^{N} w_{ik} [8\mathbb{E}\{\mathbf{x}_{k}\mathbf{x}_{k}^{T}\} + 4(\mathbb{E}\{\|\mathbf{x}_{k}\|^{2}\})]$ solution space. Estimating probability dis- $-D_{ik}^2$ ], $\Theta_i = (\alpha_i^0, \mathbf{h}_i, \mathbf{H}_i, \hat{\mathbf{h}}_i)$ tribution over solution space feasible when 1: initialize the parameters  $\Theta$  of  $\mathbf{P}^0(\mathbf{X}|\Theta)$  randomly data distributions cannot be estimated. **PC** & Norm Cut: k = 2, G = (V, E),while change of KL divergence  $\mathcal{D}^{KL} > \varepsilon$  do  $Ncut(A, B) = \frac{\text{cut}(A, B)}{\text{assoc}(A, V)} + \frac{\text{cut}(A, B)}{\text{assoc}(B, V)}$ Compute the statistics  $\Phi_i$  from the expectations  $\{\mathbb{E}\{\mathbf{x}_k\}, \mathbb{E}\{\mathbf{x}_k\mathbf{x}_k^T\}, \mathbb{E}\{\|\mathbf{x}_k\|^2\mathbf{x}_k\} : 1 \leq k \leq n, \ k \neq i\}$ , taken w.r.t.  $\mathbf{P}^0(\mathbf{X}|\Theta)$  Minimize  $\mathcal{D}^{\mathrm{KL}}(\mathbf{P}^0(\mathbf{X}|\Theta)\|\mathbf{P}^{G(\mathbf{X})})$  w.r.t.  $\Theta_i$ 11:  $T \leftarrow \eta T$ ,  $0 < \eta < 1$ 

> **Model Selection for Clustering** Validation Methods: 1) procedures and concepts for quantitative and objective assessment of clustering solutions. 2) evaluate specific quality measure. 3) external (compare with ground-



 $+ \mathbf{h}_i^T \frac{\partial \mathbb{E}\{\mathbf{x}_i\}^T}{\partial \theta_{in}} + T \frac{\partial}{\partial \theta_{ip}} \mathbb{E}\{\log q_i\}, \quad 1 \le i \le n$ 

 $\hat{\mathbf{h}}_i = -8 \sum_{k=1}^{N} w_{ik} \mathbb{E}\{\mathbf{x}_k\}, \quad \alpha_i^0 = 2 \sum_{k=1}^{N} w_{ik}$ 

Second descent in the interpolation regime when the training error vanishes and the generalization error decays with a capacity increase. Complexity MS: assume

model-based clustering, problem  $\rightarrow$  log-like diverges for vanishing variance. Strategy  $\rightarrow$  add regularization to neg log-like. **Oc-**

cam's razor: choose model with shortest description of the data  $\rightarrow$  MDL, BIC **MDL:** minimize description length  $-\log p(\mathbf{X}|\Theta_k) - \log p(\Theta_k)$  (-data-model).

Asymptot approx (-neg log-like + penalty)  $\tilde{k} \in \operatorname{argmin} \left( -\log(p(\mathbf{X} \mid \tilde{\Theta}_k)) + \frac{1}{2}k' \log n \right)$ 

 $\bar{l}(\theta) = \frac{1}{n} \log p(X|\theta, M) = \frac{1}{n} \sum_{i} \log p(x_i|\theta, M)$  $\bar{l}(\theta) = \bar{l}(\hat{\theta}) - \frac{1}{2}(\hat{\theta} - \theta)^{\top} \left(-\frac{\partial^2 \bar{l}(\theta)}{\partial \theta \partial \theta^{\top}}_{\theta = \hat{\theta}}\right) (\theta - \hat{\theta})$  $p(X|M) \propto C \cdot \exp(l(\hat{\theta}))(\frac{2\pi}{n})^{\frac{k}{2}} |\mathcal{I}(\hat{\theta})|^{-\frac{1}{2}}$ 

sets from same source should be similar. Stable solut. transferred to second data (same distribution) at minimal model misfit Two sample scenario: 1) Draw two data sets from same source 2) Cluster both data sets 3) Compute disagreement. In Practice: only one dataset avaible, 1) Estimate expected agreement by resampling 2) Cluster entire dataset with optimal k. How to measure disagreement of two clustering c and c' on disjoint data? Extend solution from X' to X with classifiers. 1) Train a predictor  $\phi_{\mathbf{Z}'}(\cdot)$  on data  $\mathbf{Z}' := (\mathbf{X}', \hat{c}(\mathbf{X}'))$ 2) Predict labels on **X** using  $\phi_{\mathbf{Z}'}$  3) Compare clustering solutions  $(\phi_{\mathbf{Z}'}(X_i))_{i \in [n]}$  and  $\hat{c}(\mathbf{X})$  on  $\mathbf{X}$ . Symmetry Breaking: problem  $\rightarrow$  labeling unique only up to  $\pi \in \mathfrak{S}_k$ .

 $p(X|M) = \exp(\log l(\hat{\theta}) - \frac{k}{2}\log(n) +$ 

O(1)) = exp $(-\frac{\text{BIC}}{2} + O(1))$ ,  $p(M|X) \propto$ 

 $p(X|M)p(M) \approx \exp(-\frac{\text{BIC}}{2})p(M)$ . MDL

and BIC are consistent as a model selection

⊕ Well-motivated model selection schemes.

→ MDL/BIC methods to model selection

rely on likelihood optimization. (not gen

Stability-based Validation if no prior

knowledge avaible → solutions on two data

applicable)  $\oplus$  Many variants,  $\ominus \lambda$  tuning.

criterion for  $n \to \infty$ .

# $d_{\tilde{E}_{i}}(\hat{c}_{k}(\mathbf{X}), \phi'_{\mathbf{Z}}(\mathbf{X}))$ In Practice: Estimate $\mathbb{E}_{\mathbf{X},\mathbf{X}'}$ by resampling. $t(\mathbf{X})$ any target labelling. Then $S_k(\hat{c}) <$

Solution: Stability index S :=expected

Hungarian method  $O(k^3)(O(n))$  pre-

processing). Final Measure for Stability:

minimal disagreement over all  $\pi \in \mathfrak{S}_k$ :

 $\mathbb{E}_{\mathbf{X}} d_{\mathfrak{G}_k}(\hat{c}_k(\mathbf{X}), t(\mathbf{X})) + \mathbb{E}_{\mathbf{X}, \mathbf{X}'} d_{\mathfrak{S}_k}(t(\mathbf{X}), \phi'_{\mathbf{Z}}(\mathbf{X}))$ Large  $S_k \to \text{not close to any target labelling}$ on average! 

⊕ Performance on experimental datasets. Stability method overlooks solution complexity. Tradeoff betw informative and stability needs quantitative eval, requiring algo validation theory.

#### Nature of DSA: train X', validation X''Substitute data-hypothesis relation with posterior distribution. How select scoring for posterior: conciseness (minimize MDL),

generalization (high score validation)

hypotheses  $\theta \in \Theta$  necessary for inference (If can rule out hypotheses before measured  $data \rightarrow exclude such hypothesis a priori)$ Generalization DL: for Gibbs distrib  $\mathbb{E}_{\theta|X'}\text{-}\log\mathbf{P}(\theta|X'') = \beta(\mathbb{E}_{\theta|X'}R(\theta,X'')\text{-}\mathcal{F}(X''))$  $X'_{\mathcal{E}}, X''_{\mathcal{E}}$  generated by same experiment  $\mathcal{E}$ . **Object:** MDL post given test data when

**Design constraints hyp**  $\Theta$ : a priori, all

$$\mathbf{P}^{\mathcal{A}}(X'_{\mathcal{E}}, X'''_{\mathcal{E}}|\varphi_{\mathcal{E}}) = \mathbf{P}^{\mathcal{A}}(X'_{\mathcal{E}}|\varphi_{\mathcal{E}})\mathbf{P}^{\mathcal{A}}(X''_{\mathcal{E}}|\varphi_{\mathcal{E}}),$$
**M2** valdata perturbation of train data (iid)
$$\mathbf{P}^{\mathcal{A}}(X'_{\mathcal{E}}, X''_{\mathcal{E}}|\varphi_{\mathcal{E}}) = \mathbf{P}^{\mathcal{A}}(X''_{\mathcal{E}}|X'_{\mathcal{E}})\mathbf{P}^{\mathcal{A}}(X'_{\mathcal{E}}|\varphi_{\mathcal{E}})$$
M2 corresponds to noisy channel transmission where random codebook vector  $X'_{\mathcal{E}}$  corrupted by channel noise  $\mathbf{P}^{\mathcal{A}}(X''_{\mathcal{E}}|X'_{\mathcal{E}}).$ 
Scale oo sample DL M1, M2  $k_{\mathcal{A}}(X''_{\mathcal{E}}, X''_{\mathcal{E}}):$ 

hvp. sampled from post given train data

M1 Train/val data cond. independent

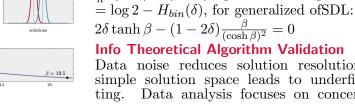
 $-\log \mathbf{P}_{\mathcal{E}}^{\mathcal{A}}(\theta|\varphi_{\mathcal{E}}) = -\log \mathbb{E}_{X_{\mathcal{E}}''|\varphi_{\mathcal{E}}} \mathbf{P}^{\mathcal{A}}(\theta|X_{\mathcal{E}}'',\varphi_{\mathcal{E}}) (\sum_{\theta \in \Theta} \frac{\mathbf{P}(\theta|X_{\mathcal{E}}')\mathbf{P}(\theta|X_{\mathcal{E}}'')}{\mathbf{P}(\theta)} \mathcal{W}(X_{\mathcal{E}}',X_{\mathcal{E}}'',\theta))] \leq$  $= -\log \mathbb{E}_{X'_{\mathcal{E}}|\varphi_{\mathcal{E}}} \mathbb{E}_{X''_{\mathcal{E}}|X'_{\mathcal{E}}} \mathbf{P}^{\mathcal{A}}(\theta|X''_{\mathcal{E}},\varphi_{\mathcal{E}}),$  $\mathbb{E}_{X_{\mathcal{E}}',X_{\mathcal{E}}''}[\log\sum_{\theta\in\Theta}\frac{\mathbf{P}(\theta|X_{\mathcal{E}}')\mathbf{P}(\theta|X_{\mathcal{E}}'')}{\mathbf{P}(\theta)}]+$ Score  $\min_{\mathcal{A}} \mathbb{E}_{X_{\mathcal{E}}', X_{\mathcal{E}}''} \mathbb{E}_{\theta \mid X_{\mathcal{E}}'} (-\log \frac{\mathbf{P}^{\mathcal{A}}(\theta \mid X_{\mathcal{E}}'')}{\mathbf{P}_{\mathcal{A}}^{\mathcal{A}}(\theta)}) \geq$  $\mathbb{E}_{X'_{\mathcal{C}}, X''_{\mathcal{C}}}[\log \max_{\theta} \{\mathcal{W}(X'_{\mathcal{E}}, X''_{\mathcal{E}}, \theta)\}]$  $\min_{\mathcal{A}} \mathbb{E}_{X_{\mathcal{E}}', X_{\mathcal{E}}''}(-\log \mathbb{E}_{\theta \mid X_{\mathcal{E}}'} \frac{\mathbf{P}^{\mathcal{A}}(\theta \mid X_{\mathcal{E}}'')}{\mathbf{P}^{\mathcal{A}}(\theta)}) \geq 0$ , with

 $\mathbb{E}_{X_{\mathcal{E}}',X_{\mathcal{E}}''}\mathbb{E}_{\theta|X_{\mathcal{E}}'}(-\log\frac{\mathbf{P}^{\mathcal{A}}(\theta|X_{\mathcal{E}}'')}{\mathbf{P}_{\hat{c}}^{\hat{c}}(\theta)})=\mathbb{E}_{X_{\varepsilon}',X_{\varepsilon}''}$ solutions  $\theta$  are suff. stat of  $X'_{\varepsilon}, X''_{\varepsilon}$ .  $\mathcal{D}(\mathbf{P}^{\mathcal{A}}(\theta|X_{\varepsilon}')\|\mathbf{P}^{\mathcal{A}}(\theta|X_{\varepsilon}'')) - \mathcal{I}(\theta;X_{\varepsilon}) \ge 0$ ming dist  $\in [0, n], x, c \in \{-1, 1\}^n$ Prob Richness: sampling hyp uniform  $d(c,x) = \sum_{i=1}^{n} \frac{1}{2} (1 - x_i c_i) = \frac{n}{2}$ from all experiments yield uniform prior

 $\pi(\theta) := \mathbb{E}_{\mathcal{E}} \mathbf{P}_{\mathcal{E}}^{\mathcal{A}}(\theta) \approx |\Theta|^{-1}.$ 

 $p(c|X) = \prod_{1}^{n} \frac{\exp(\beta x_i c_i)}{\sum_{c} \exp(\beta \sum_{1}^{n} x_i c_i)}$  $\min_{\mathcal{A}} \mathcal{D}(\pi(\theta)||\Theta|^{-1}) = \log |\Theta| - \max_{\mathcal{A}} H_{\pi}(\theta)$ Post. selection:  $\min_{\mathcal{A}}(\mathbb{E}_{X_c',X_c''}\mathbb{E}_{\theta|X_c'}(-\log$  $\prod_{1}^{n} \frac{\exp(\beta x_{i} c_{i})}{2 \cosh(\beta x_{i})}, Z^{2} = 2^{2n} (\cosh \beta)^{2n}$  $\frac{\mathbf{P}^{\mathcal{A}}(\theta|X_{\mathcal{E}}^{\prime\prime})}{\mathbf{P}_{\mathcal{E}}^{\mathcal{A}}(\theta)}) + \lambda \mathcal{D}(\pi(\theta) |||\Theta|^{-1})) \ge -\max_{\mathcal{A}}(\lambda$ Expected alignment  $\mathbb{E}_{c|x} \frac{1}{n} \sum_{i=1}^{n} x_i c_i$  $S_k(\hat{c}) = \mathbb{E}_{\mathbf{X},\mathbf{X}'}(\min_{\pi \in \mathfrak{S}_k} \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}_{\{\hat{c}_k(\mathbf{X})_i \neq \pi \circ \phi_{\mathbf{z}'}(X_i)\}}) H_{\pi}(\theta) - \lambda \log |\Theta| + \mathbb{E}_{X',X''} \log k_{\mathcal{A}}(X'_{\mathcal{E}}, X''_{\mathcal{E}})) \geq -\tanh \beta, \text{ Channel noise } \delta := \frac{1}{n} \sum_{i \leq n} \mathbb{I}_{\{x'_i \neq x''_i\}} \mathbb{I}_{\{x'_i \neq x''_i\}} + \sum_{e^{-\beta x''_i}} \mathbb{I}_{\{x'_i \neq x''_i\}} \mathbb{I}_{\{x'_i \neq x''_i\}} + \mathbb{I}_{\{x'_i \neq x''_$ 

> $\geq \max \mathbb{E}_{X'_{\mathcal{E}}, X''_{\mathcal{E}}} \log(k_{\mathcal{A}}(X'_{\mathcal{E}}, X''_{\mathcal{E}})), H_{\pi}(\theta) =$  $+e^{\beta(x_i'+x_i'')c_i} = \frac{1}{7^2}2^n(\cosh 2\beta)^{n(1-\delta)}$  $\log |\Theta|$ , Kernel topo concept, part ordering  $I = \mathbb{E}_{x',x''} \log |c| k(x',x'') \propto n(1-\delta).$ normalized desc length  $\mathbb{E}_{\theta|X_{\mathcal{E}}'}(-\log \frac{\mathbf{p}^{\mathcal{A}}(\theta|X_{\mathcal{E}}'')}{\mathbf{p}_{\mathcal{E}}^{\mathcal{A}}(\theta)})$  $\log \cosh 2\beta - 2n \log \cosh \beta \rightarrow \frac{\partial I}{\partial \beta}$



 $\mathbb{E}_{X',X''}\log k_{\mathcal{A}}\left(X',X''\right) \ge \frac{1}{L}\sum_{l\le L}\log k_{\mathcal{A}}\left(X'_{l},X''_{l}\right) - \text{ penalty}$ signal. *Objective:* rank algorithms based 2: Estimate the optimal empirical posterior distribution: on signal sensitivity and noise robustness. 3:  $\mathbf{P}_{\mathrm{opt}}^{\mathcal{A}}(. \mid .) \in \arg \max_{\mathcal{A}} \left( \frac{1}{L} \sum_{l < L} \log k_{\mathcal{A}} \left( X'_{l}, X''_{l} \right) - \text{ penalty} \right)$ 4: Sample hypotheses  $\theta \sim \mathbf{P}_{\mathrm{opt}}^{\mathcal{A}}(\theta \mid X''')$  from optimized Algorithm 3 Structure Validation IT 1: Sample a hypothesis  $\tilde{c} \sim p^{\mathcal{A}}(c \mid \mathbf{X})$ 2: **for** j = 1, ..., M **do** 

from "posterior agreement"  $\theta \sim \mathbf{P}_{\text{opt}}^{\mathcal{A}}(\theta \mid X') \mathbf{P}_{\text{opt}}^{\mathcal{A}}(\theta \mid X'')$  $\mathbf{P}(X_{\mathcal{E}}', X_{\mathcal{E}}'') = \sum_{\theta} \mathbf{P}(X_{\mathcal{E}}', X_{\mathcal{E}}''|\theta)\mathbf{P}(\theta) =$  $\sum_{\theta} \frac{\mathbf{P}(X_{\mathcal{E}}', X_{\mathcal{E}}''|\theta)}{\mathbf{P}(X_{\mathcal{E}}'|\theta)\mathbf{P}(X_{\mathcal{E}}''|\theta)} \mathbf{P}(X_{\mathcal{E}}'|\theta) \mathbf{P}(X_{\mathcal{E}}''|\theta) \mathbf{P}(\theta) =$  $\sum_{\theta} \frac{\mathbf{P}(X_{\mathcal{E}}', X_{\mathcal{E}}''|\theta)}{\mathbf{P}(X_{\mathcal{E}}'|\theta)\mathbf{P}(X_{\mathcal{E}}''|\theta)} \frac{\mathbf{P}(\theta|X_{\mathcal{E}}')}{\mathbf{P}(\theta)} \mathbf{P}(X_{\mathcal{E}}') \frac{\mathbf{P}(\theta|X_{\mathcal{E}}'')}{\mathbf{P}(\theta)}$ 

Algorithm 2 Posterior Selection Algorithm

posterior  $\mathbf{P}_{\text{opt}}^{\mathcal{A}}$  given future data X''' or

1: Derive empirical lower bound on PA kernel score

 $\cdot \mathbf{P}(X_{\mathcal{E}}'')\mathbf{P}(\theta), \ \mathcal{W}(X_{\mathcal{E}}', X_{\mathcal{E}}'', \theta) \le \mathbf{P}(X_{\mathcal{E}}')\mathbf{P}(X_{\mathcal{E}}'')$  $\sum_{\theta \in \Theta} \frac{\mathbf{P}(\theta|X_{\mathcal{E}}')\mathbf{P}(\theta|X_{\mathcal{E}}'')}{\mathbf{P}(\theta)} \max_{\theta} \{ \mathcal{W}(X_{\mathcal{E}}', X_{\mathcal{E}}'', \theta) \}$ Insert in Mutual information  $\mathcal{I}(X'_{\varepsilon}, X''_{\varepsilon}) =$  $\mathbb{E}_{X_{\mathcal{E}}', X_{\mathcal{E}}''}[\log \frac{\mathbf{P}(X_{\mathcal{E}}', X_{\mathcal{E}}'')}{\mathbf{P}(X_{\mathcal{E}}')\mathbf{P}(X_{\mathcal{E}}'')}] = \mathbb{E}_{X_{\mathcal{E}}', X_{\mathcal{E}}''}[\log$ 

 $MI \rightarrow weighted version of PA bounded$ above by PA and constant (vanishes if Binary sym channel: minimize Ham- $\frac{1}{2}\sum_{i=1}^{n}x_{i}c_{i}, R^{\text{Ham}}(c,x) = -\sum_{i=1}^{n}x_{i}c_{i}$ 

sender sender

problem generator

 $\max_{\mathcal{A}} \mathbb{E}_{X',X''} \log(\frac{\exp(\lambda H_{\pi}(\theta))}{|\Theta|^{\lambda}} k_{\mathcal{A}}(X'_{\mathcal{E}}, X''_{\mathcal{E}})) \leq 1^{\frac{1}{2}|\mathbf{x}' - \mathbf{x}''|} = n\delta, k(x', x'') = \sum_{c} \frac{e^{-\beta x'_{c}}}{Z'} \frac{e^{-\beta x''_{c}}}{Z'} \frac{e^{-\beta x''_{c}}}{Z''}$  $= \frac{1}{Z^2} \sum_{c} \prod_{i} e^{-\beta(x_i' + x_i'')c_i} = \frac{1}{Z^2} \prod_{i} e^{-\beta(x_i' + x_i'')}$ 

 $\frac{1}{n}I(\beta^{opt}) = (1-\delta)\log\cosh 2\beta - 2\log\cosh \beta$ 

Info Theoretical Algorithm Validation

 $\cosh \beta = \sqrt{\frac{1}{2}(\cosh 2\beta + 1)} = (2\delta)^{-1/2}$ 

Data noise reduces solution resolution;

simple solution space leads to underfit-

5: end for 6: **return** Codebook  $\mathcal{T} := \{\tilde{c}_1, \dots, \tilde{c}_M\}$ Approximation sets (AS): data in high dim space, measure sensitivity sol sets to noise. Coding with sets of approximate

> rankings: define set code problems. Com**munication** by AS: estimate coding error problem generator PG

trated data distributions with signals and

noise. Worst case analysis neglects the

Select random transformation  $\tau_i \in \mathbb{T}$ 

Define code vector  $\tilde{c}_i \sim p^A (c \mid \tau_i \circ \mathbf{X})$ 

receiver

receiver

**Algorithm 4** Communication by approximation sets 1: Sender sends transformation  $\tau_s$  to problem generator Problem generator sends a new problem with transformed indices to receiver without revealing  $\tau_s$ . 3: Receiver identifies transformation  $\hat{\tau}$  by comparing approximation sets.

Approximate Sorting: given N objects  $o_1...o_i...o_N$ , rank them based on pairwise noisy comparisons represented by dataset X, with  $X_{ij} = 1$  if  $o_i < o_j$ , 0 else,  $X_{ii} = 0$ and  $X_{ij} = 1 - X_{ji} \ \forall i, j \neq i$ , feasible solu-

tions = all permutations c over items, where  $c_i = \ell = \text{position (rank) of obj } o_i$  $\mathcal{R}^{sort}(c|X) := |\{(i,j)|X_{ij} = 1 \text{ but } c_i > c_i\}|$ Let M assignment matrix with  $M_{il} = 1$  if  $o_i$ gets rank l, 0 else,  $\sum_{\ell i} M_{i\ell} = 1$ , item/rank get unique rank/item,  $M(i) = \ell \Leftrightarrow M_{i\ell} = 1$  $\mathcal{R}^{\text{sort}}(M|X) = \sum_{i} \sum_{j} \sum_{\ell} \sum_{\bar{\ell}>\ell} X_{ij} M_{i\bar{\ell}} M_{j\ell}$ 

MFA:  $q_{i\ell} := \frac{e^{-\beta \mathcal{E}_{i\ell}}}{\sum_{h} e^{-\beta \mathcal{E}_{ih}}}, \ Q(M|\mathcal{E}) = q_{1M(1)}$  $q_{2M(2)}\cdots q_{NM(N)}, \, \mathcal{E}_{i\ell} = \mathbb{E}_{M\sim Q_{i\to \ell}}[\mathcal{R}^{\text{sort}}],$ in before equation notation means  $o_i$  to rank l, Q satisfies this constraint, not both ting. Data analysis focuses on concen- C1)  $X_{ij} = 1 \Rightarrow i \to \ell$  and  $j \to \underline{\ell}$  with  $\underline{\ell} < \ell$ 

 $=\sum_{il} M_{il}(\mathcal{E}_{il} + \lambda_l) + \text{cst}, \ \lambda_l \text{ from } \sum_i q_{i\ell} = 1$ **sMBP:** given G = (V, E, W), select subset of nodes U, find min bisection for U. If  $|U|0\Theta(n^{2/7}) \to \text{NP-hard}$ . **REM:** given  $N = \Theta(\exp(n))$  states  $J \in \mathcal{H}$ , i.i.d. score  $(R(c, \mathbf{X}))$  values score(J)  $\sim \mathcal{N}(0, \sqrt{n})$ .  $\approx \exp(-|\mathcal{H}|\exp(-\mu^2/4))$ Find  $\widehat{J}_{\max} = \arg \max_{J \in \mathcal{H}} \operatorname{score}(J)$ , model max disordered and without structure for searching  $n^s = \Theta(n^{2/7})$ . By construction, different solutions J', J'' do not share common parameters (statistical independent) sMBP is lower/upper bounded by REM:  $\lim_{n\to\infty} \frac{\mathbb{E}[\log Z(\beta,\mathbf{X})] + \hat{\beta}\mu\sqrt{N\log m}}{\log m}$  $=1+\frac{\hat{\beta}^2\sigma^2}{2}$  if  $\hat{\beta}\sigma<\sqrt{2}$  or  $=\hat{\beta}\sigma\sqrt{2}$  (else) Generalization capacity of sMBP for noise perturbed random graph: X' = X + $\delta \mathbf{X}', \dot{\mathbf{X}}'' = \mathbf{X} + \delta \mathbf{X}'', \gamma = \sigma/\tilde{\sigma}, 2 \text{ transitions}$  $\lim_{n\to\infty} \frac{\mathbb{E}_{X,\delta X',\delta X''} \log(|\mathcal{C}|\hat{k}_{\beta}(X',X''))}{\log m}$  $\eta(\hat{\beta}) = \begin{cases} (\hat{\beta}\tilde{\sigma})^2, & \hat{\beta}\tilde{\sigma} < \frac{\sqrt{2}}{\sqrt{4+2\gamma^2}} \\ \hat{\beta}\tilde{\sigma}\sqrt{2}\sqrt{4+2\gamma^2} - (\hat{\beta}\tilde{\sigma})^2\left(1+\gamma^2\right) - 1, & \frac{\sqrt{2}}{\sqrt{4+2\gamma^2}} \leq \hat{\beta}\tilde{\sigma} < \frac{\sqrt{2}}{\sqrt{1+\gamma^2}} \\ \hat{\beta}\tilde{\sigma}\sqrt{2}\left(\sqrt{4+2\gamma^2} - 2\sqrt{1+\gamma^2}\right) + 1, & \frac{\sqrt{2}}{\sqrt{1+\gamma^2}} \leq \hat{\beta}\tilde{\sigma} \end{cases}$ REM has no information for searching  $\rightarrow$ evaluate  $M = 2^n$  cost values. Random sMBP, CDP  $\approx$  REM (free E gen. func.) Learning and algorithmic complexity Strategy for combinatorial search: 1) Define concept- and structurally simple comb. problem P1 2) Define reference prob. P2 where exhaustive search is optimal 3) Study relation betw. P1 and P2. **PREM** (P2): given  $N = O(\exp(n))$  states  $J \in \mathcal{H}$  with scores  $X_J \sim \mathcal{N}(X \mid 0, \sigma^2)$ define planted state  $I^* \sim \mathcal{N}(X|\mu, 1)$ , find state  $J_{\max} = \arg \max_{J \in \mathcal{H} \cup I^*} \operatorname{score}(J)$ . Signal: Bias  $\mu$ , unbiased scores act as observation noise. Minimal bias  $\mu_0$  for recovery in probability? (Unlimited positive bias can't improve recovery beyond exhaustive search due to lack of shared information with neighboring states) Recover prob:  $\mathbf{P}_{\mathcal{X}}(\max_{J \in \mathcal{H} \setminus \{I^{\star}\}} X_J < X_{I^{\star}}) \stackrel{n \uparrow \infty}{\longrightarrow} 1$ 

C2)  $X_{ii} = 1 \Rightarrow i \to \ell$  and  $i \to \ell$  with  $\bar{\ell} > \ell$ 

C3)  $X_{ab} = 1 \Rightarrow a \to \overline{\ell} \text{ and } b \to \ell \text{ w/ } \ell < \overline{\ell}$ 

 $\mathcal{E}_{i\ell} = \sum_{j} \sum_{\ell < \ell} X_{ij} q_{j\underline{\ell}} + \sum_{j} \sum_{\overline{\ell} < \ell} X_{ji} q_{j\overline{\ell}}$ 

 $+\sum_{a\neq i}\sum_{b\neq i}X_{ab}\sum_{\ell}\sum_{\overline{\ell}>\ell}q_{a\overline{\ell}}q_{b\underline{\ell}}$ , const

 $\mathcal{R}_{fix}^{MF}(M|\mathcal{E}) = \sum_{i,l} M_{i\ell} \mathcal{E}_{i\ell} + \sum_{\ell} \lambda_{\ell} (\sum_{i} M_{i\ell} - 1)$ 

 $\frac{1}{u}e^{-u^2/2}, d\mathcal{N}(z) = \frac{1}{\sqrt{2\pi}}\exp(-\frac{z^2}{2})dz$  $(*) \leq |\mathcal{D}(I^*)| \leq (*) \cdot (k - h + 1),$ Planted sub-hypergraph (P1): Hypothesis J is set of k indices  $J = \{j_1, \dots, j_k\} \subset$  $\{1,\ldots,n\} =: [n], \mathcal{H} = \{J \subset [n] : |J| = k\}$  $|\mathcal{H}| = {n \choose k} < {ne \choose k}^k$ , sol  $I^* = \{i_1^*, \dots, i_k^*\}$ ters of J are biased and Bin(k,h) - Bin(l,h)are unbiased. If total bias much small than Subsets H of h items assigned score  $X_H, H = \{j_1, \ldots, j_h\}$  Scores  $X_H$  are data of planted sub-hypergraph recovery.  $\operatorname{score}(J) = \sum_{H \subset J: |H| = h} X_H$ . All proper subsets H of planted sol  $I^*$  are biased.  $X_{H} = \left\{ \begin{array}{ll} \mu + \xi_{H} & H \subset I^{\star} \\ \xi_{H} & H \not\subset I^{\star} \end{array}, \xi_{H} \sim \mathcal{N}(0, \sigma^{2}) \right.$ **Note:** J defined by Bin(k,h) parameters  $X_H$ . When h increases, localize planted solution  $I^*$  by using Bin(n,h) RV as parameters (localization of solutions). **Interaction degree** h: h = 1 sort the  $X_i$  $|k - l_{\perp}|(k - l_{\perp} + 1)| - \ln \text{Bin}(n, h)|$ values, select k largest score(J) =  $\sum_{i \in J} X_i$ , h=2 find k-clique with only biased edges,  $score(J) = \sum_{(i,j)\in J\times J} X_{i,j}, \ h \geq 3 \text{ sub-}$ hypergraph recovery, h = k identify set  $J = \arg \max_{J \subset [n]} X_J$  employing exhaustive search of Bin(n, k) states,  $score(J) = X_J$ . Increasing  $h \to k$  localizes influence planted For case  $\mathcal{D}(I^*) = \mathcal{D}^{\text{eft}}(I^*)$  with  $l_{\perp} =$ 

solution  $I^*$  up to single state at expense of increasing amount of (random) data. **REM recovery:** k sub-hypergraph recovery with h = k interaction suppresses parameter sharing and eliminates statistical dependence between solutions. This independence implies REM behavior since all of the Bin(n, k) subsets of size k of n items are characterized by individual score value.

Success prob. to recover Planted REM:  $\mathbf{P}(\widehat{J} = I^{\star}) \ge \exp(-\exp(\ln|\mathcal{H}| - \frac{\mu^2}{4}))$ 0/1 behaviour, threshold  $\mu_0 = 2\sqrt{\ln |\mathcal{H}|}$ :  $\lim_{n \uparrow \infty} \mathbf{P}(\widehat{J} = I^*) = 1 \text{ if } \mu > \mu_0, = 0 \text{ else}$  $\mathbf{P}(\hat{J} = I^{\star}) = \mathbb{E}_{X_{I^{\star}}} \mathbf{P}(\hat{J} = I^{\star} | X_{I^{\star}}) = \mathbb{E}_{X_{I^{\star}}}$ 

$$\begin{aligned} \mathbf{P}(\hat{J} = I^{\star}) &= \mathbb{E}_{X_{I^{\star}}} \mathbf{P}(\hat{J} = I^{\star} | X_{I^{\star}}) = \mathbb{E}_{X_{I^{\star}}} \\ \mathbf{P}(\bigwedge_{J \neq I^{\star}} X_{J} < X_{I^{\star}} | X_{I^{\star}}) &= \mathbb{E}_{X_{I^{\star}}} \prod_{J \neq I^{\star}} \\ \mathbf{P}(X_{J} < X_{I^{\star}} | X_{I^{\star}}) &= \mathbb{E}_{X_{I^{\star}}} (\int_{-\infty}^{X_{I^{\star}}} d\mathcal{N}(z) \\ |^{\mathcal{H}|-1} &= \mathbb{E}_{X_{I^{\star}}} (1 - \int_{X_{I^{\star}}}^{\infty} d\mathcal{N}(z))^{|\mathcal{H}|-1} \geq (1 - \mathbb{E}_{X_{I^{\star}}} \int_{X_{I^{\star}}}^{\infty} d\mathcal{N}(z))^{|\mathcal{H}|} \geq (1 - \mathbb{E}_{X_{I^{\star}}} \frac{\mathcal{N}(X_{I^{\star}})}{X_{I^{\star}}})^{|\mathcal{H}|} \\ \mathbb{E}_{X_{I^{\star}}} \int_{X_{I^{\star}}}^{\infty} d\mathcal{N}(z)^{|\mathcal{H}|} \geq (1 - \mathbb{E}_{X_{I^{\star}}} \frac{\mathcal{N}(X_{I^{\star}})}{X_{I^{\star}}})^{|\mathcal{H}|} \end{aligned}$$
5: Prove absense of effective statistical tests to amplify asymptotically vanishing search information.

$$\text{How many states share param with planted solution } I^{\star} ? \text{ Assume } |J \cap I^{\star}| = l \geq l$$
set of solution  $I^{\star}$ ? Set of solution  $I^{\star}$  se

$$\begin{aligned} \mathbf{P}(X_J < X_{I^\star} | X_{I^\star}) &= \mathbb{E}_{X_{I^\star}} (\int_{-\infty}^{\infty} d\mathcal{N}(z)) & solution \ I^\star? \quad \text{Assume} \ |J \cap I^\star| = l \geq \\ )^{|\mathcal{H}|-1} &= \mathbb{E}_{X_{I^\star}} (1 - \int_{X_{I^\star}}^{\infty} d\mathcal{N}(z))^{|\mathcal{H}|-1} \geq (1 - h \Rightarrow \operatorname{Bin}(k,l) \cdot \operatorname{Bin}(n-k,n-l). \quad \mathcal{D}(I^\star) \\ \mathbb{E}_{X_{I^\star}} \int_{X_{I^\star}}^{\infty} d\mathcal{N}(z)^{|\mathcal{H}|} &\geq (1 - \mathbb{E}_{X_{I^\star}} \frac{\mathcal{N}(X_{I^\star})}{X_{I^\star}})^{|\mathcal{H}|} & \text{set of solu } J \text{ statistically dependent on } I^\star \\ &\approx \exp(-|\mathcal{H}| \exp(-\mu^2/4)) & \text{solution } I^\star = l \geq \\ &\text{set of solu } J \text{ statistically dependent on } I^\star \\ &\text{share at least } 1 \text{ param}). \quad \operatorname{Let} |\mathcal{D}(I^\star)| = \\ &\approx \exp(-|\mathcal{H}| \exp(-\mu^2/4)) & \sum_{l=h}^k \operatorname{Bin}(k,l) \operatorname{Bin}(n-k,n-l), k = n^\alpha, 0 < \\ &\text{Note: } \frac{1}{u}e^{-u^2/2}(1+u^{-2}) \leq \int_u^\infty e^{-z^2/2}dz \leq \\ &\alpha < \frac{1}{2}, \operatorname{Bin}(k,h) \cdot \operatorname{Bin}(n-k,n-h), \text{ then} \end{aligned}$$

Algorithm 5 Hypergraph recovery problem

1: Define spectrum of hypergraph recovery prob

 $(1 \le h \le k)$  with increased localization of solutions. 2: Characterize the statistical dependencies of solutions.

3: Compare the community detection case  $h = \mathcal{O}(n^0)$  with REM as limit case h = k for  $k = n^{\alpha}, 0 < \alpha < \frac{1}{2}$ 

4: Estimate number of effectively independent solutions to measure the computational complexity of the search problem.

amplify asymptotically vanishing search information.

*Proof:* upper bound holds since (\*) monotonically decreases in l for  $k = o(\sqrt{n})$ . Effective independence: if sol J shares l > h items with  $I^*$ , then Bin(l, h) parame-

 $|\mathcal{D}^{\text{eft}}(I^{\star})| = \sum_{l=l}^{k} \text{Bin}(k, l) \cdot \text{Bin}(n - k,$  $(k-l) \approx \operatorname{Bin}(k, l_{\perp}) \operatorname{Bin}(n-k, k-l_{\perp})(k-l_{\perp}+1)$ Sub hyp det rate:  $\mathfrak{R} = \ln \frac{|\mathcal{H}|}{|\mathcal{D}^{\text{eff}}(I^*)||\mathcal{X}|}$ 

with  $r = \sum_{\nu=1}^{\infty} \frac{1}{\nu(\nu+1)} \left(\frac{b}{a}\right)^{\nu} +$ 

 $l_{\perp}$ )  $(\ln \frac{n-k}{k-l_{\perp}} + 1) - \ln(k-l_{\perp} + 1) - h(\ln \frac{n}{k} + 1)$ The terms linear in  $l_{\perp}$  define the leading contributions in n (since the terms linear in k vanish asymptotically), i.  $-l_{\perp}(\ln\frac{k}{l_{\perp}}+1)+l_{\perp}(\ln\frac{n-k}{k-l_{\perp}}+1) = l_{\perp}\ln\frac{(n-k)l_{\perp}}{(k-l_{\perp})k} \ge l_{\perp}\ln\frac{nl_{\perp}}{k^2} = (1+\beta-2\alpha)n^{\beta}\ln n = \mathcal{O}(n^{\beta}\ln n)$ The sum of terms proportional to k is negative; therefore, we bound its absolute value from above, i.e.,  $-k(\ln\frac{n}{k}+1)+k(\ln\frac{n-k}{k-l_1}+1)+kr(n,k) = k\ln\frac{k(n-k)}{n(k-l_1)}+kr(n,k) = k\ln\frac{1-k/n}{1-l_1/k}+kr(n,k)$ 

h, rate scale polynomial in n with  $\Re$  =

 $\mathcal{O}(h \ln n)$ ,  $\oplus$  refined if  $h = \mathcal{O}(n^{\gamma})$ . Proof:

 $k \ge k(\ln \frac{n}{k} + 1) - kr(n, k) - l_{\perp}(\ln \frac{k}{l_{\perp}} + 1) - (k - 1)$ 

since  $kr(n,k)\sim \frac{k^2}{n}=O(n^{2\alpha-1})\to 0$  for  $2\alpha<1$ . Collecting all the terms yields the final rate  $\Re \ge l_{\perp} \ln \frac{nl_{\perp}}{l_{\perp}^2} - l_{\perp} - h(\ln \frac{n}{l_{\perp}} + 1) - \ln(k - l_{\perp} + 1) = O(n^{\beta} \ln n)$ since the positive term  $l_{\perp} \ln \frac{nl_{\perp}}{k^2} = \mathcal{O}(n^{\beta} \ln n)$  dominates the negative terms that scale as  $l_{\perp} = \mathcal{O}(n^{\beta})$  and it also dominates  $h(\ln \frac{n}{k} + 1) + \ln(k - l_{\perp} + 1) = \mathcal{O}(\ln n)$  in this scaling limit  $h = \mathcal{O}(1)$ .

independent on  $I^*, (|J'' \cap I^*| < h); J'$  and

J'' are stat independent  $(|J' \cap J''| < h)$ 

 $= k \sum_{-1}^{\infty} \frac{1}{\nu} \left( \frac{l_{\perp}^{\nu}}{k^{\nu}} - \frac{k^{\nu}}{n^{\nu}} \right) + kr(n,k) = l_{\perp} - \frac{k^{2}}{n} + \sum_{-1}^{\infty} \frac{k}{\nu} \left( \frac{l_{\perp}^{\nu}}{k^{\nu}} - \frac{k^{\nu}}{n^{\nu}} \right) + kr(n,k) \leq l_{\perp} + kr(n,k) = \mathcal{O}(n^{\beta}),$ 

**Exponential scaling:**  $h = O(n^{\gamma}), 0 < \gamma \le$  $\beta < \alpha, |\mathcal{X}| = \operatorname{Bin}(n, h) = O(n^{(n^{\gamma})}), l_{\perp} = \omega h$ with  $\omega = O(1)$ ,  $\Re \geq l_{\perp} \ln \frac{nl_{\perp}}{l_{\perp}^2} - l_{\perp} - h(\ln \frac{n}{h} +$ 

1)  $-\ln(k-l_{\perp}+1) \cong \omega h \ln \frac{n\omega h}{k^2} - \omega h$  $h(\ln \frac{n}{h} + 1), \frac{\Re}{h \ln n} \ge \omega(1 + \gamma - 2\alpha) - 1 + \gamma +$  $\frac{\omega(\ln \omega - 1) - 1}{\ln n} > 0, \ \alpha - \gamma = \frac{\psi}{\ln n}, \omega - 1 = \frac{\tau}{\ln n}$ 

standard dev,  $(\text{Bin}(l,h)\mu \ll \sqrt{\text{Bin}(k,h)\sigma})$ , Rate is positive in asymptotic limit ( $\mathcal{R} \geq$ then cant distinguish betw sol with l shared  $n^{\gamma}$ ) for  $\tau > 2\frac{\psi+1}{1-\alpha} \Rightarrow \frac{\Re}{h \ln n} \geq 0$ , so items and independent solution due to fluc- $\omega > 1 + \frac{2}{1-\alpha}(\alpha - \gamma) + \frac{2}{(1-\alpha)\ln n}$ tuations. Assume that overlap  $h \leq l \leq l_{\perp}$  $(l_{\perp} \text{ cutoff parameter})$  too weak to significant Small overlap: sol J' weakly stat dependependence, # effectively dependent states: dent on  $I^{\star}$   $(|\vec{J'} \cap I^{\star}| = l > h)$ ; solJ'' stat

 $\operatorname{score}\left(J'\right) = \sum_{H \subset J' \cap I^*} X_H + \sum_{\tilde{H} \subset J' \wedge \tilde{H} \not\subseteq I^*} X_{\tilde{H}} \sim \mathcal{N}\left(\left(\begin{array}{c} l \\ h \end{array}\right) \mu, \left(\begin{array}{c} k \\ h \end{array}\right) \sigma^2\right)$  $\geq \ln \text{Bin}(n,k) - \ln [\text{Bin}(k,l_{\perp})] \cdot \text{Bin}(n-k,l_{\perp})$ score  $(J'') = \sum_{H=J''} X_H \sim \mathcal{N}\left(0, \begin{pmatrix} k \\ h \end{pmatrix} \sigma^2\right)$ If  $\mathfrak{R} = \mathcal{O}(n^{\beta})$ , exponentially many indescore  $(J', J'') \in \text{Bin}(l, h)\mu \pm \sqrt{\text{Bin}(k, h)\sigma}$ 

select maximal overlap  $l_{\perp}$  as  $Bin(l_{\perp}, h) =$ pendent states that define REM and this REM is exponentially larger than the num- $\epsilon \sqrt{\operatorname{Bin}(k,h)} \frac{\sigma}{\mu} \to l_{\perp} = \sqrt{k} (\epsilon \frac{\sigma}{\mu})^{\frac{1}{h}}$ , Induce ber of parameters! Since a REM requires subsampled hyp class  $\mathcal{H}^{\Delta}$ , with  $|\mathcal{H}^{\Delta}| =$ exhaustive search, conclude that searching for planted sub-hypergraph is exponentially  $\frac{|\mathcal{H}|}{|\mathcal{D}^{\text{eff}}(I^{\star})|} = \mathcal{O}(n \exp(n^{\beta})), \text{ REM recovery}$ more expensive than testing. **Stirling:** 

condition:  $\frac{\mu}{\sigma} > 2\sqrt{\ln |\mathcal{H}^{\Delta}|}, \beta, \alpha = \frac{1}{7}, \frac{1}{3}$  $n! = \sqrt{2\pi n} (\frac{n}{e})^n \cdot (1 + \frac{1}{12n} + \mathcal{O}(n^{-2}))$  $\ln \operatorname{Bin}(a,b) \stackrel{\circ}{=} b \ln \frac{a}{b} + b(1-r) \le b(\ln \frac{a}{b} + 1)$ 

 $\frac{1}{2b}\ln 2\pi b \left(1-\frac{b}{a}\right) = \mathcal{O}\left(\max\left\{\frac{b}{a},\frac{1}{b}\right\}\right)$ **Recovery Theo:** if  $k = n^{\alpha}$ ,  $l_{\perp} = n^{\beta}$ , h =

 $\mathcal{O}(n^0), 2\alpha < 1$ , then  $\Re \geq l_{\perp} \ln \frac{l_{\perp} n}{l_{\perp}^2} - l_{\perp} - l_{\perp}$  $h(\ln \frac{n}{h} + 1) - \ln(k - l_{\perp} + 1) = \mathcal{O}(n^{\beta} \ln n)$ 

$$\begin{split} l_{\perp} &= n^{\beta} < \sqrt{k} (\frac{\epsilon}{2\sqrt{\ln|\mathcal{H}^{\Delta}|}})^{\frac{1}{h}} = \mathcal{O}(n^{\frac{\alpha}{2}}n^{-\frac{\beta}{2h}}) \\ \text{Ising Model, } N &= \# \text{ pixel, } \lambda \& J_{ij} \geq 0 \\ E(\sigma|\mathbf{h}) &= -\lambda \sum_{i=1}^{N} h_i \sigma_i - \sum_{\langle i,j \rangle} J_{ij} \sigma_i \sigma_j, \end{split}$$

 $\mathbf{h} = \{h_i\} \text{ noisy img, } \boldsymbol{\sigma} = \{\sigma_i, h_i\} (\sigma_i \in$  $\{-1,1\}$ ) denoised img (sol), like, prior MCMC:  $p_i(\boldsymbol{\sigma}) = \exp(-\beta \max[0, \Delta E_i(\boldsymbol{\sigma})])$ 

 $P(\boldsymbol{\sigma}, \boldsymbol{\sigma}') = \frac{1}{N} p_i(\boldsymbol{\sigma})$  if  $\boldsymbol{\sigma}' = \boldsymbol{\sigma}^{(i)}$  for some  $i_i = 1 - \frac{1}{N} \sum_{i=1}^{N} p_i(\boldsymbol{\sigma}) \text{ if } \boldsymbol{\sigma}' = \boldsymbol{\sigma} \text{ , else } 0.$  Irreducible and stationary, detailed balance hold, periodic (if  $E(\sigma) = E$  for all state, period 2, only case  $\rightarrow$  no loop = E const)  $Periodic \ p\text{-}prior: -\sum_{i=1}^{N-p} \sigma_i \sigma_{i+p}$  (E is sum of p 1-periodic Ising energies)

## **Algorithm 1** Metropolis-Hastings 1: Define $\{q(\cdot \mid c)\}_{c \in C}$ s.t $\mathcal{G}_q$ is connected, $q(c \mid c) > 0$ $2: c_0 \leftarrow \$$ 3: **for** $t = 1, 2, \dots$ **do** $\tilde{c} \stackrel{\$}{\leftarrow} q(\cdot \mid c_{t-1})$ $b \stackrel{\$}{\leftarrow} \operatorname{Ber}(\min\{1, \frac{q(c_{t-1}|\tilde{c})p(\tilde{c})}{q(\tilde{c}|c_{t-1})p(c_{t-1})}\})$ if b = 1 then Set $c_t = \tilde{c}$ (Accept the proposal) Set $c_t = c_{t-1}$ (Reject the proposal) end if 10: $t \leftarrow t + 1$ 12: end for

#### Algorithm 2 Posterior Selection Algorithm

```
1: Derive empirical lower bound on PA kernel score
    \mathbb{E}_{X',X''}\log k_{\mathcal{A}}(X',X'') \ge \frac{1}{L}\sum_{l\le L}\log k_{\mathcal{A}}(X'_l,X''_l) penalty
```

- 2: Estimate the optimal empirical posterior distribution:
- 3:  $\mathbf{P}_{\mathrm{opt}}^{\mathcal{A}}(. \mid .) \in \arg \max_{\mathcal{A}} \left(\frac{1}{L} \sum_{l \leq L} \log k_{\mathcal{A}}(X_{l}', X_{l}'') \text{ penalty}\right)$ 4: Sample hypotheses  $\theta \sim \mathbf{P}_{\mathrm{opt}}^{\mathcal{A}}(\theta \mid X''')$  from optimized posterior  $\mathbf{P}_{\text{opt}}^{\mathcal{A}}$  given future data X''' or from "posterior agreement"  $\theta \sim \mathbf{P}_{\text{opt}}^{\mathcal{A}}(\theta \mid X') \mathbf{P}_{\text{opt}}^{\mathcal{A}}(\theta \mid X'')$

# Algorithm 3 Structure Validation IT

- 1: Sample a hypothesis  $\tilde{c} \sim p^{\mathcal{A}}(c \mid \mathbf{X})$ 2: **for** j = 1, ..., M **do**
- Select random transformation  $\tau_i \in \mathbb{T}$
- Define code vector  $\tilde{c}_i \sim p^{\mathcal{A}}(c \mid \tau_i \circ \mathbf{X})$
- 5: end for
- 6: **return** Codebook  $\mathcal{T} := \{\tilde{c}_1, \dots, \tilde{c}_M\}$

# Algorithm 4 Communication by approximation sets

- 1: Sender sends transformation  $\tau_s$  to problem generator
- 2: Problem generator sends a new problem with transformed indices to receiver without revealing  $\tau_s$ .
- 3: Receiver identifies transformation  $\hat{\tau}$  by comparing approximation sets.

$$\eta(\hat{\beta}) = \begin{cases} (\hat{\beta}\tilde{\sigma})^2, & \hat{\beta}\tilde{\sigma} < \frac{\sqrt{2}}{\sqrt{4+2\gamma^2}} \\ \hat{\beta}\tilde{\sigma}\sqrt{2}\sqrt{4+2\gamma^2} - (\hat{\beta}\tilde{\sigma})^2\left(1+\gamma^2\right) - 1, & \frac{\sqrt{2}}{\sqrt{4+2\gamma^2}} \leq \hat{\beta}\tilde{\sigma} < \frac{\sqrt{2}}{\sqrt{1+\gamma^2}} \\ \hat{\beta}\tilde{\sigma}\sqrt{2}\left(\sqrt{4+2\gamma^2} - 2\sqrt{1+\gamma^2}\right) + 1, & \frac{\sqrt{2}}{\sqrt{1+\gamma^2}} \leq \hat{\beta}\tilde{\sigma} \end{cases}$$

### Algorithm 5 Hypergraph recovery problem

- 1: Define spectrum of hypergraph recovery prob  $(1 \le h \le k)$  with increased localization of solutions.
- 2: Characterize the statistical dependencies of solutions.
- 3: Compare the community detection case  $h = \mathcal{O}(n^0)$  with REM as limit case h = k for  $k = n^{\alpha}, 0 < \alpha < \frac{1}{2}$ .
- 4: Estimate number of effectively independent solutions to measure the computational complexity of the search problem.
- 5: Prove absense of effective statistical tests to amplify asymptotically vanishing search information.

score 
$$(J') = \sum_{H \subset J' \cap I^*} X_H + \sum_{\tilde{H} \subset J' \wedge \tilde{H} \not\subset I^*} X_{\tilde{H}} \sim \mathcal{N}\left(\begin{pmatrix} l \\ h \end{pmatrix} \mu, \begin{pmatrix} k \\ h \end{pmatrix} \sigma^2\right)$$
  
score  $(J'') = \sum_{H \subset J''} X_H \sim \mathcal{N}\left(0, \begin{pmatrix} k \\ h \end{pmatrix} \sigma^2\right)$