



# ; cZg\ n#8VhZY HZhYj VaBViZci I gVchedgj [dgJ chj eZgk hZY Fd'ci 9æj Y 9db eaZi 'dc



Hj ^V^9j ^ i ] ^Gj ^ (" i VZZY 7cl Vg'(" @c\ O] Vc\' " D X' 8VgZh' '7j hig/vaVc DVi 'dcVal c kZgh'n ( : ViV, ' #9i 7HE

## æigdyj Xi 'dc

/, s- B, YHH> > % N~H> } L~> ^L...L%~> , ~, N / nL, } L^~¥ B ~^sAY ~n, ~Y} L^, Y%> >...>B> , ~%~^, A, B%~Y, ~>Cn> , ~ >Yn} L~LH^L>s¥ L^B &§ sLHA¥C^L E s-n>-nL , BB¥%~ >-H>BtYs% , ~^L%Y , ~ ^>E ... s- B, YH%~L nL-L^> ¥%~>Hs-B } ...L



f snY'L ~-B } ...L^L ... s- B, YH%~ ...L%

7 ~%~.L^C%~H... s- B, YHB } ...L , ~ >§ % s-NL^ "pL Ep, L nL, } L^~¥, N>...^ > , A^B^, A%~ C> , ~ E sp, Y^ ^L^Yss-n...^ > B } ...L^L B ^L%~ -HL-BL

## C di kVi 'dc

- Ž L~L^> CL ) , HL s-n fl^%~n } L^p, H LCL^>nL%~ , -L " , , -L HL^L^ } s-%~B } >...s-n , B } ...L^L >...^ > %>...L ž , ELCL^ ^LB CL^s-n } %~n nL, } L^~d%~B ^L%~ -H%~ , ~L " , } >~¥%~ Bp>%~B } >...s-n %~EL ... , ... %~H "pL T^%~Y~%~.L^C%~HB } ...L , ~ } L^p, H A>%~H , ~ nL-L^> CL } , HL s-n
- &>L~" 5>~%~.~ : L >%~} L "p> ^L...L%~> , ~%~N>...^ > ... s- B, YH>-Hs%~>HB } ...L^L N^ } %~L B, %~s- "pL >L~" %~BL %~EL HL%~ -LH> >L~" %~BL L~L^n¥ A>%~H } , HL fl.) s- >-L-B, HL^ HLB HL^>BpsLB^Y^L >§ s-n , L>~>... , A>Ass¥Hs%~sAY , ~ B, ~Hs, ~LH, ~ "pL ...^ > %~>...L L-B Hs-n
- 2L%~Y> 3> } ...s-n 5, ^>s- "pL >L~" B, HL ^>~%~.~ } , HYL >-H "pL L-B, HL^ HLB HL^ ~L^E, ^y ws- ¥ EL s- , HYL > ^L%~Y> %~ } ...s-n %~>Ln¥ E pL^L "pL ^L%~Y> B>..Y^L%~pL H, } >s- n>... AL^ELL~ ...^ > >-HB } ...L^L %~>...L >L~" %~BL%

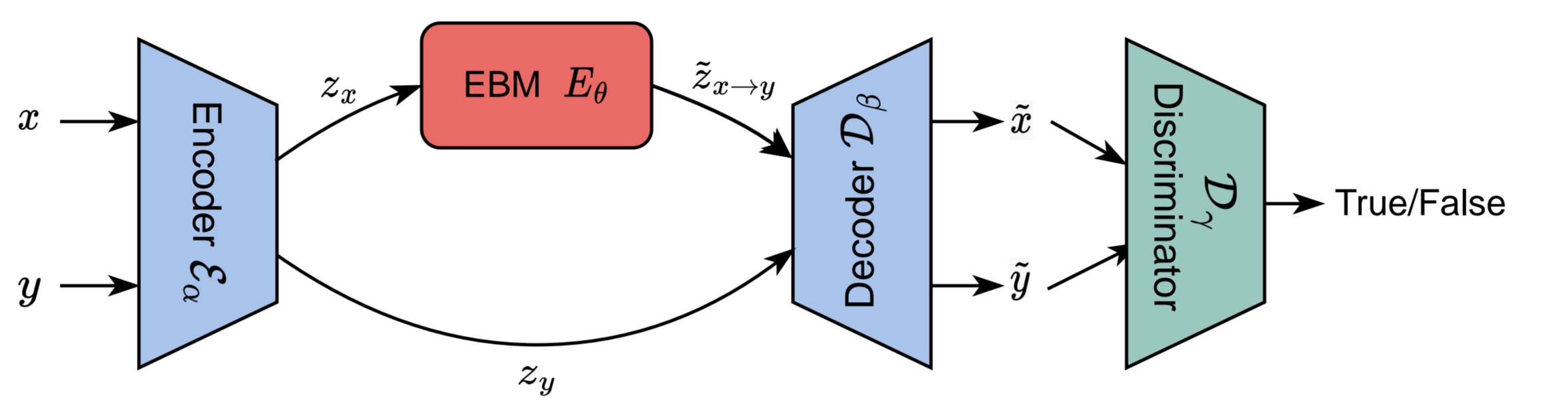
## 9dcigWj i 'dc

- , Y^ } >s- B ~^sAY , ~%~L %~ } >^sLHAL , E
- : L ... , ... %~>~ , CL L~L^n¥ A>%~H >L~" ^>~%~.~ } LBp>~%~ L~>A s-n nL-L^> CL } , HL s-n , N^pL Y~%~.L^C%~H... s- B, YHB } ...L , ~ >%~N^ "pL T^%~ } L
- : L ...L%~> ^L%~Y> %~ } ...s-n %~>Ln¥ "p> " > , E %~ws- ^>s-s-n, N> >L~" %~BL fl.) >-H >-L-B, HL^ HLB HL^ N^ "pL T^%~ } L
- fl.a.L^ž L~> ^L%~%~s-HB>L "p> , Y^ } , HL ~ , , ~ ¥>BpsCL%~%~L , N^pL >~ ...L^L^ } >-BL , ~ %~>pL B 3p>...L^L^ >-H^L> E , ^H %~55" 3B>~\* L^ ) >^L^ , ~ / H> >%~%~sAY^ %~%~ B>...A L , NnL-L^> -n L...>A L Y~BL^>~s-¥ } >...%

## =ZcZgVi kZ C dYZæc\ <gVb ZI dg

&L" x X >-Hy Y AL %~ } ...L%~B, } "pL ...> >-HB, } ...L^L ... s- B, YHH, } >s- ^L%~dB CL ¥ , Y^ } , HL B ~%~%~N^p^LL } >s- ...>^%~> } L ¥

>-L-B, HL^ N^ ... s- B, YHB, HL L^>B , ~ >-H>HLB, HL^ N^ ... s- B, YH^LB, ~%~YB , ~ > >L~" %~BL L~L^n¥ A>%~H } , HL E sp L~L^n¥ N~B , ~ E " , T "pL B, HL n>...AL^ELL~ "pL ...^ > ... s- B, YH>-Hs%~B ^L%~ -Hs-n B } ...L , ~ >... s- H, } >s- Hs%~ s- , ^ , >BpsCL >HCL^%~s L>~s-n



f snY'L ) , HL , CL^CL E

## BViZci# eVXZ ; cZg\ n8VhZY C dYZaVcY HZhYj Vai Vb eaç\

~ p> L~nL%~ -H%~Y , ~, N>...¥s-nfl.) N^ Y~%~.L^C%~H... s- B, YHB } ...L , ~

5, HLT~L "pL B ~Hs , ~> Hs%~sAY , ~ , N^pL B, } ...L^L %~>...L >L~" B, HL EL Y%~>-L~L^n¥ N~B , ~ E (zy, zx) ...> } L^L^sLHA¥>HLL...~LY> ~L^E, ^y , } >... "pL B HL ...>s (zy, zx) " , > %~> > "p> } L>%~L%~pLs B } ...> Ass¥ ž , ELCL^ s- "pL Y~%~.L^C%~H%~ -n EL >L s-B>...A L , NhsLB^ ¥ } , HL s-n "pL B, } ...> Ass¥, NzX >-H Zy HYL " , >By, N...sLH%~ } ...L%~ "L~> CL ¥ EL } , HL "pL B ~Hs , ~> Hs%~sAY , ~ , N^pL ^L%~Y> rxy s-%~LH^ ^L...L%~ -n "pL Hs%~sAY , ~ n>...AL^ELL~ "pL >L~" %~BL , N^pL "E, H, } >s-%~%

$$p(r_{xy}/z_x) = \frac{\int p(r_{xy}, z_x) p(r_{xy}, z_x) dz_x}{\int p(r_{xy}, z_x) dz_x} = \frac{\exp[-E(r_{xy}, z_x)]}{Z(r_{xy})}$$

\$ s- 5>s-s-n, Nfl.) >-H "pL fl-B HL^ / LB HL^ f^> } LE, ^y

ž CL~ "pL >A, CL N^ } Y > , ~ >L%~Y> rxy B>~ AL nL-L^>LHN, } "pL B ~Hs , ~> Hs%~YAY , ~ A¥ %~ } ...s-n E sp &>-nLCS- H¥> } B%~pL- >B } ...L^L %~>...L B HL ž\_x y B>~ AL , A^>s-LH >%~

$$\tilde{z}_x y = z_x + (r_{xy})$$

ž L^L EL >...¥ "pL %~ ...n^>H~ , ..L^> , ~ ( : ) , >C, sY~N Hs-n "pL &>-nLCS- H¥> } B%~L^> , ~ >-Hs-C, CS-n "pL %~B ~H, "HL^ n^>H~ , N^rxy s- N^Y^L n^>H~ B } ..Y^> , ~ ) , ^L, CL^ "pL ...> } L^L^ , N^pL L~L^n¥ N~B , ~ B>~ AL Y..H>LH E sp n^>H~ " HLT-LH >%~

$$= \frac{1}{N} \sum_{i=1}^N E_{\tilde{z}_x y} p[-E(\tilde{z}_x^i y)] - E_{z_y} p_{z_y}[-E(z_y)] + C,$$

E pL^L C %~ B ~%~> E pBp B>~ AL sn- , ^LH H¥^s-n ^>s-s-n

## ; mæZgb Zcih

5>A L 3p>...L^ , } ...L , ~ ^L%~%~N%~.L^C%~H Y...L^ "p^LL^ , E %~>-H Y~%~.L^C%~H , EL^TCL^ , E %~ } L^p, H%~> 3p>...L^ L^ 5pL ~Y } AL^%~ E ~ >L^ 2^ / %~>LHA¥10^4

) L^p, H	^ Cn / >-L^ >As-L^ ~ >^ p>s &> } ...3, N>5>A L , >
/ fl/*	
f, Hs-n^ L	
/~*	
/B /B	
3p>...L^~C	
^ >SL^ >	
, Y^%~	

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Öæi

šæ [ ]

Væi^

f snY'L 1 Y>s> CL 2L%~ , ~ "pL 3p>...L^ L"

, Y^ N> } LE, ^y B>~ ... , C^HL Y~BL^>~s-¥ } >...%~> %~ } >^sL "pL %~ Bp>%~B^¥

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šf,

Pi^8

f snY'L 7-BL^>~s-¥ } >...%~pL T^%~>-H%~B ~H^ , E %~> E ...> , A%~C> , ~%~>-H^pLs B } ...L^L n^, Y~H^Y^p >-H^pL "pSH>-H N^Y^p , E %~> E "E, CL E %~N^Y~BL^>~s-¥ } >...%