Inference for latent variable Energy Based Models (EBMs)

Toy example, the ellipse

INFERENCE
Un-supervised learning

Un-conditional case

Training samples

$$\alpha = 1.5$$
$$\beta = 2$$

$$\boldsymbol{y} = \begin{bmatrix} \rho_1(x)\cos(\theta) + \varepsilon \\ \rho_2(x)\sin(\theta) + \varepsilon \end{bmatrix}$$

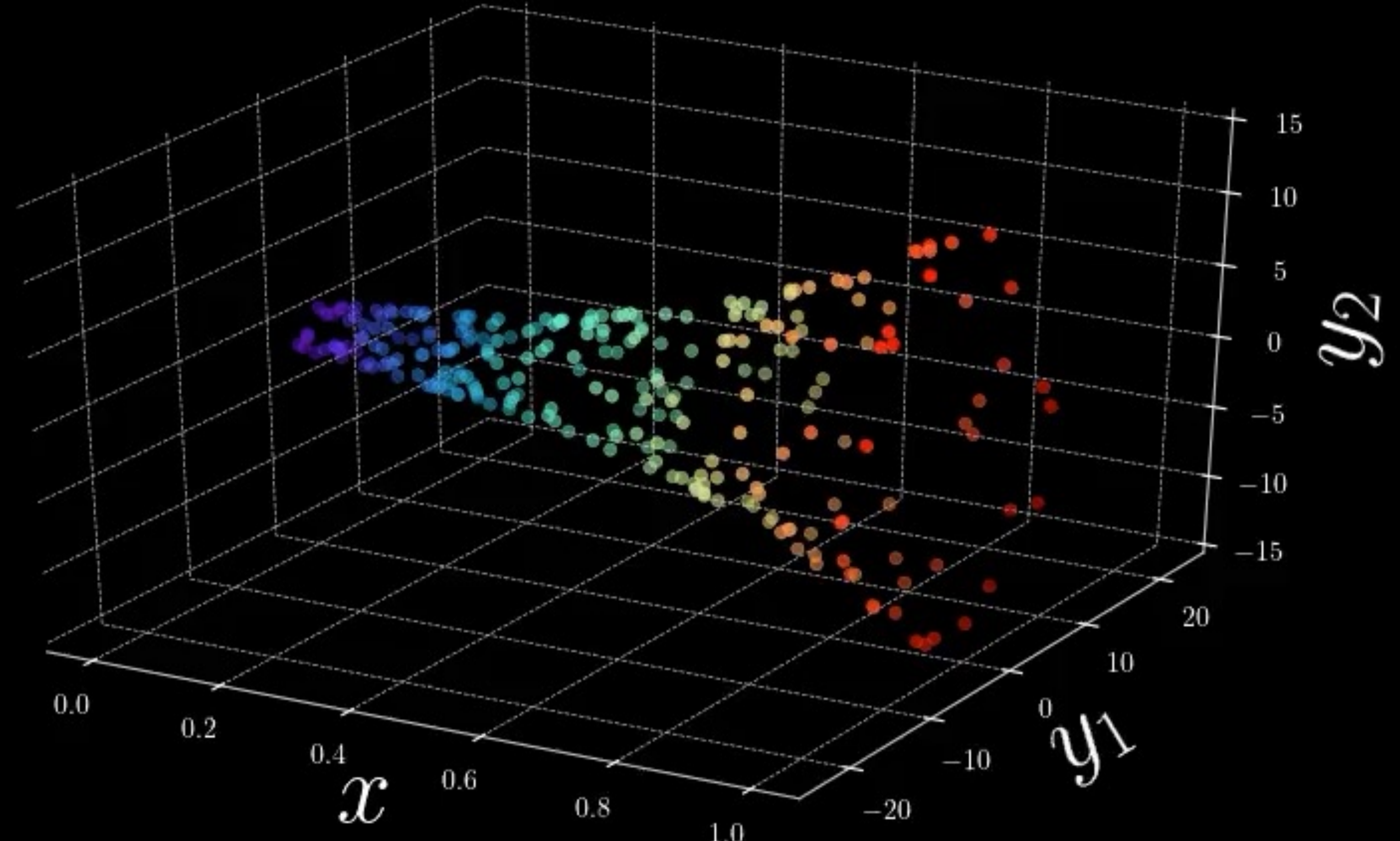
$$\rho : \mathbb{R} \to \mathbb{R}^2$$

$$x \mapsto \begin{bmatrix} \alpha x + \beta(1-x) \\ \beta x + \alpha(1-x) \end{bmatrix} \cdot \exp(2x)$$

$$x \sim \mathcal{U}(0,1)$$

$$\theta \sim \mathcal{U}(0,2\pi)$$

$$\varepsilon \sim \mathcal{N}\left[0, \left(\tfrac{1}{20}\right)^2\right]$$



Training samples

$$\alpha = 1.5$$

$$\beta = 2$$

$$\boldsymbol{Y} = [\boldsymbol{y}^{(1)}, \ldots, \boldsymbol{y}^{(24)}]$$

$$\boldsymbol{y} = \begin{bmatrix} \cancelto{2}{\rho_1(x)} \cos(\theta) + \varepsilon \\ \cancelto{1.5}{\rho_2(x)} \sin(\theta) + \varepsilon \end{bmatrix}$$

$$\rho : \mathbb{R} \to \mathbb{R}^2$$

$$x \mapsto \begin{bmatrix} \alpha x + \beta(1-x) \\ \beta x + \alpha(1-x) \end{bmatrix} \cdot \exp(2x)$$

$$x \sim \cancelto{0}{\mathcal{U}(0,1)}$$

$$\theta \sim \mathcal{U}(0, 2\pi)$$

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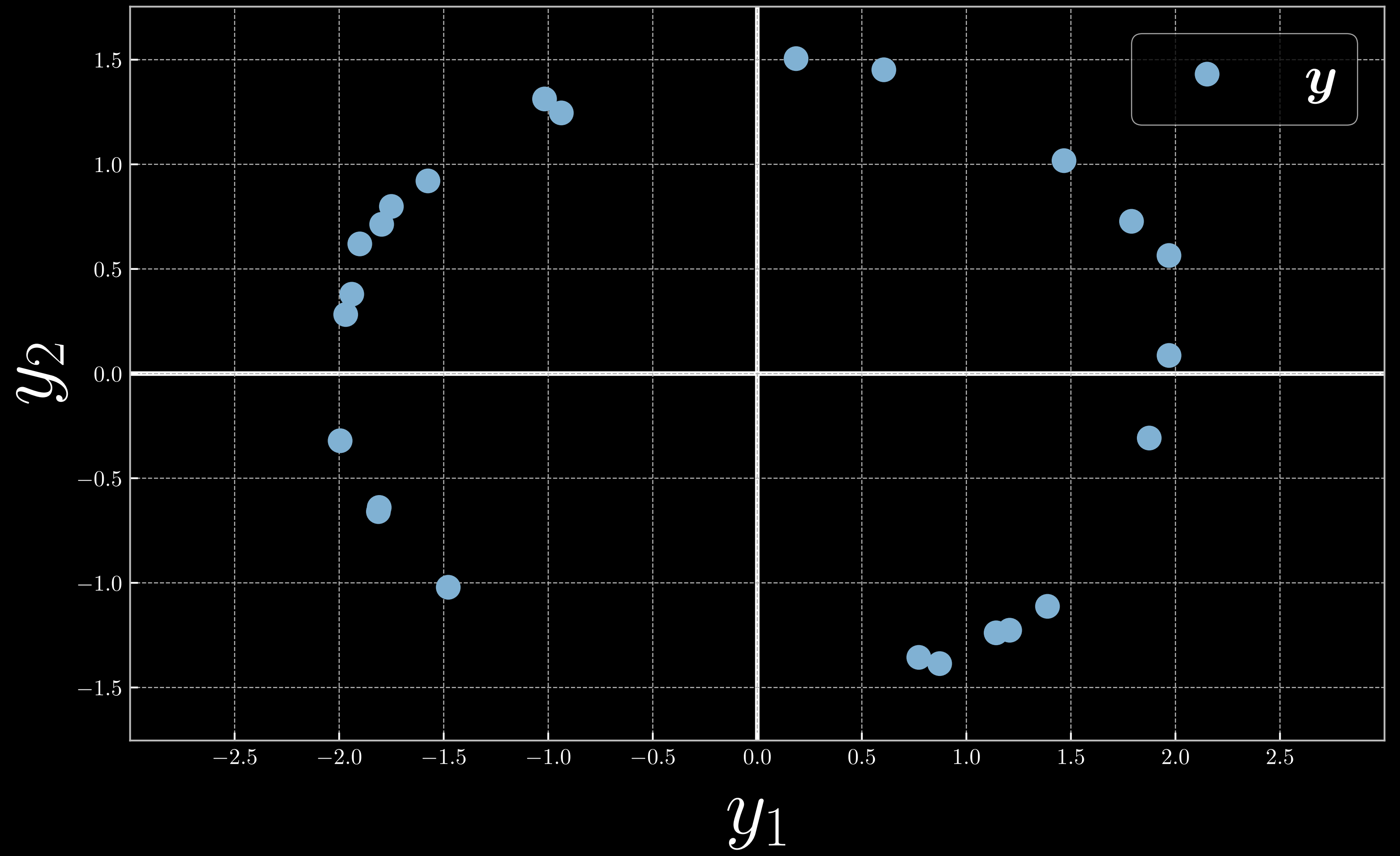
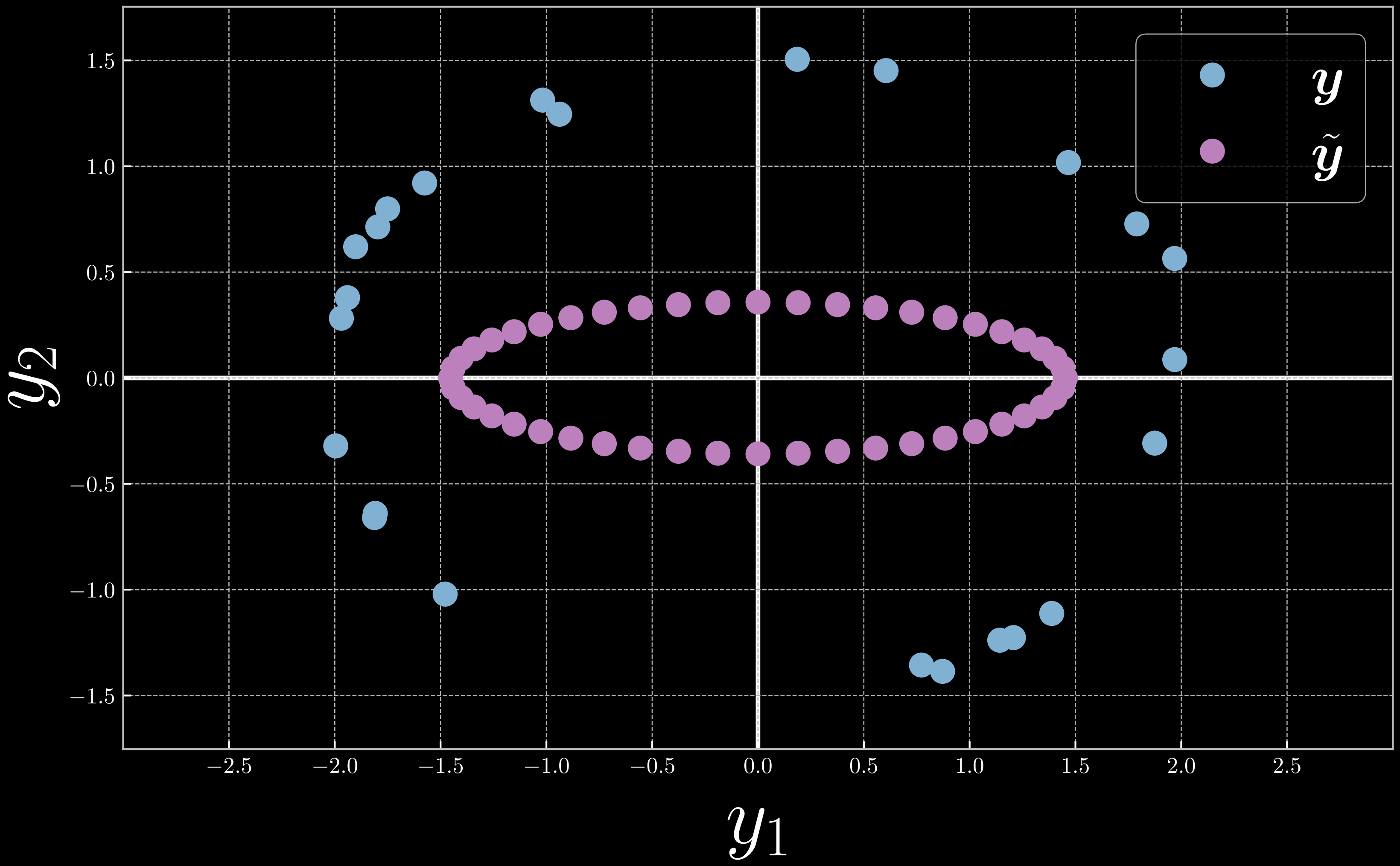
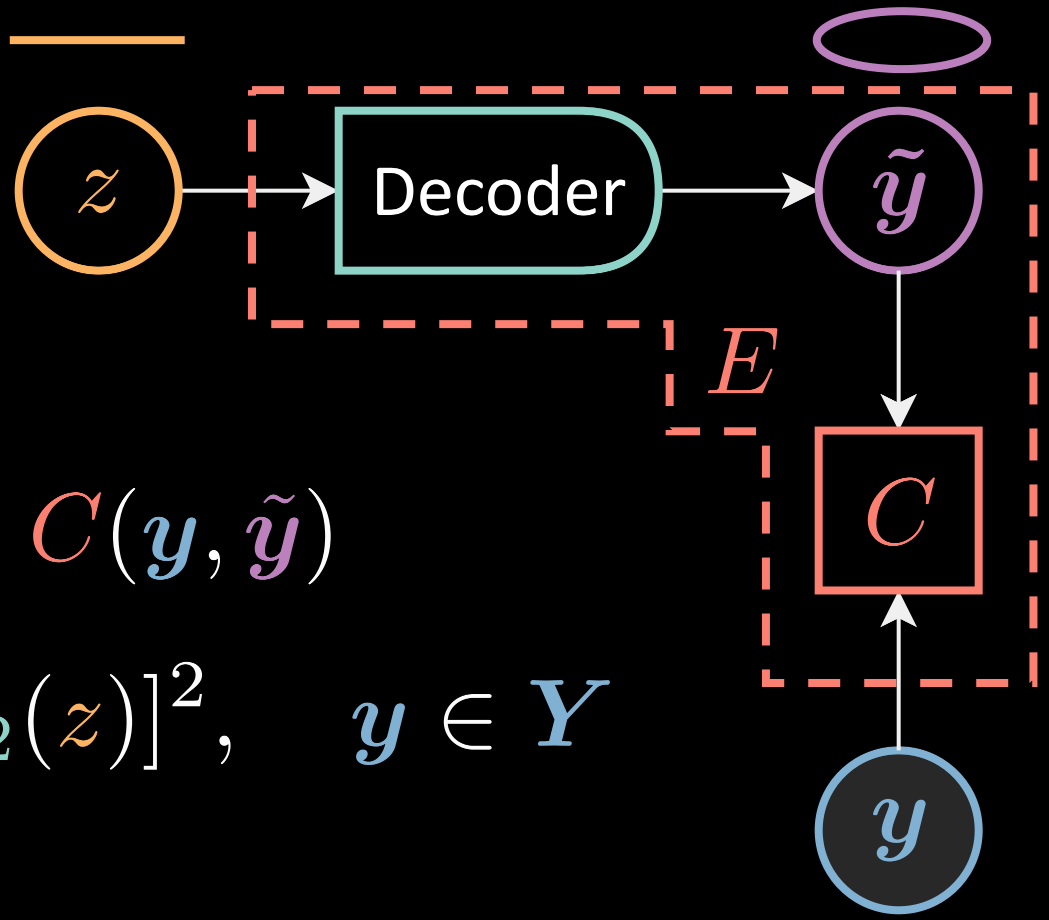


Untrained model manifold



$$z = \left[0 : \frac{\pi}{24} : 2\pi\right[$$

Energy function $E(\boldsymbol{y}, z)$



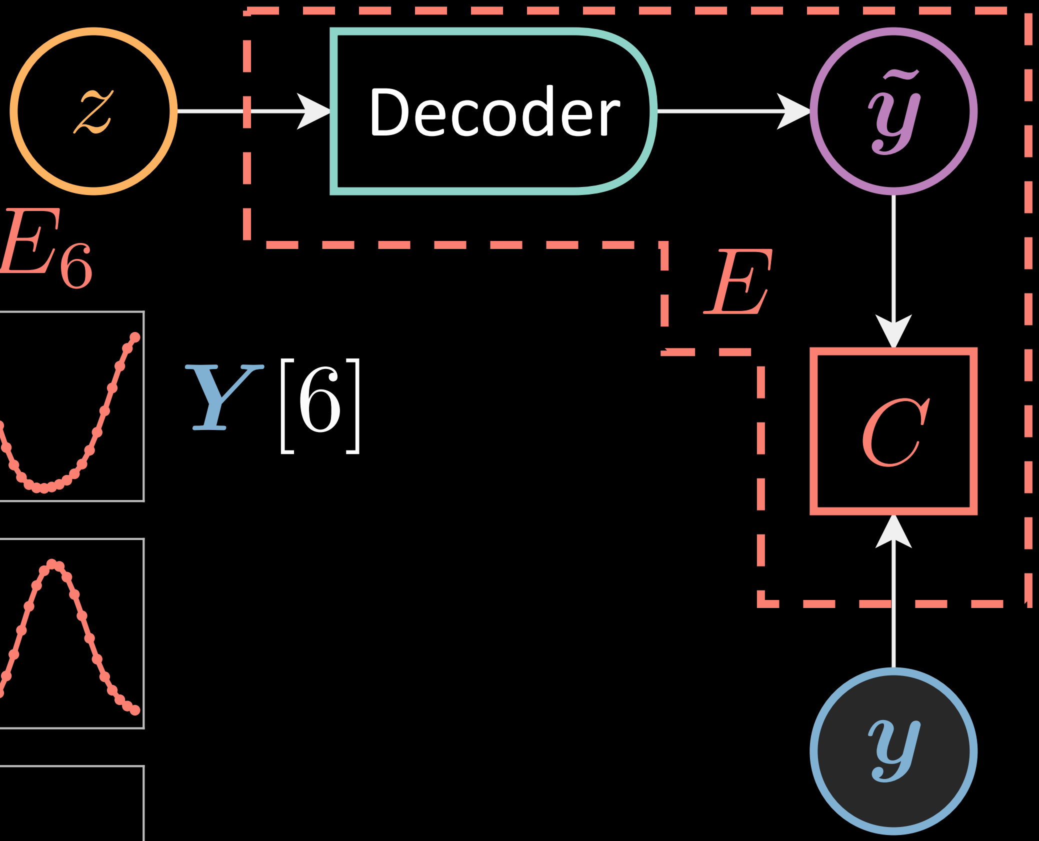
$$C(\boldsymbol{y}, \tilde{\boldsymbol{y}}) = \|\tilde{\boldsymbol{y}} - \boldsymbol{y}\|^2 \qquad E(\boldsymbol{y}, z) = C(\boldsymbol{y}, \tilde{\boldsymbol{y}})$$

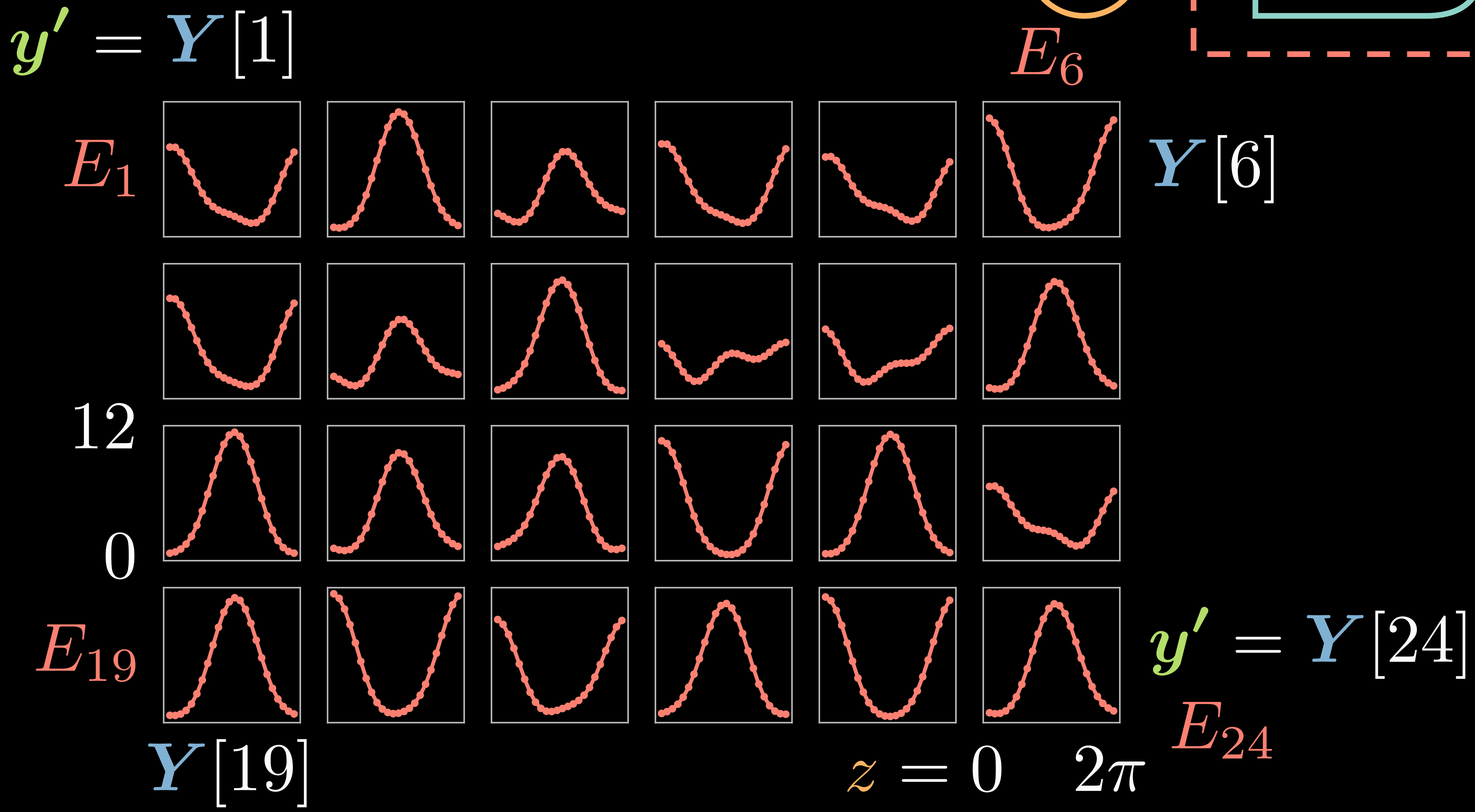
$$E(\boldsymbol{y}, z) = [y_1 - g_1(z)]^2 + [y_2 - g_2(z)]^2, \quad \boldsymbol{y} \in \boldsymbol{Y}$$

$$g = \begin{bmatrix} g_1 & g_2 \end{bmatrix}^\top : \mathbb{R} \to \mathbb{R}^2$$

$$z \mapsto \begin{bmatrix} w_1 \cos(z) & w_2 \sin(z) \end{bmatrix}^\top$$

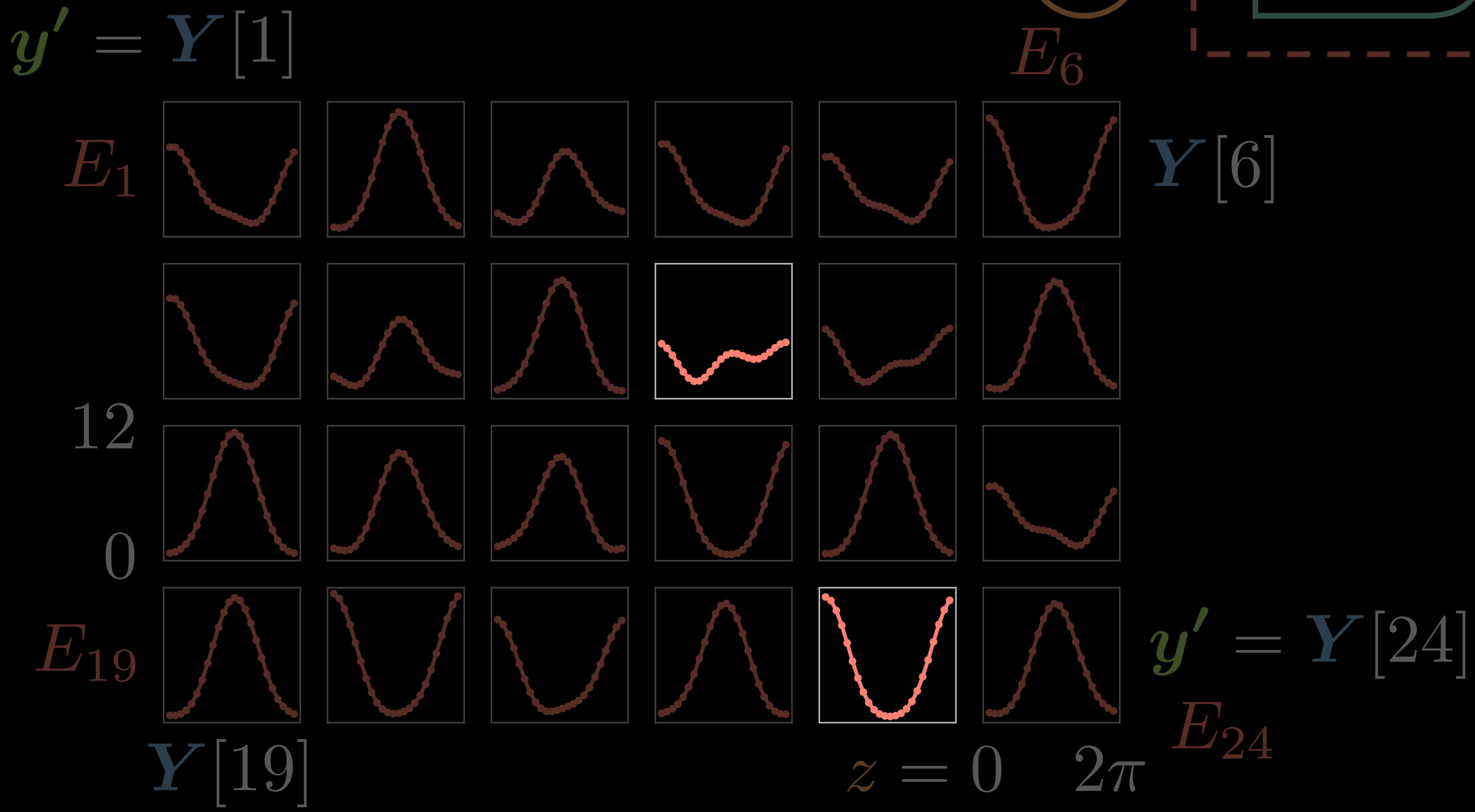
Energy function $E(\boldsymbol{y}, z)$

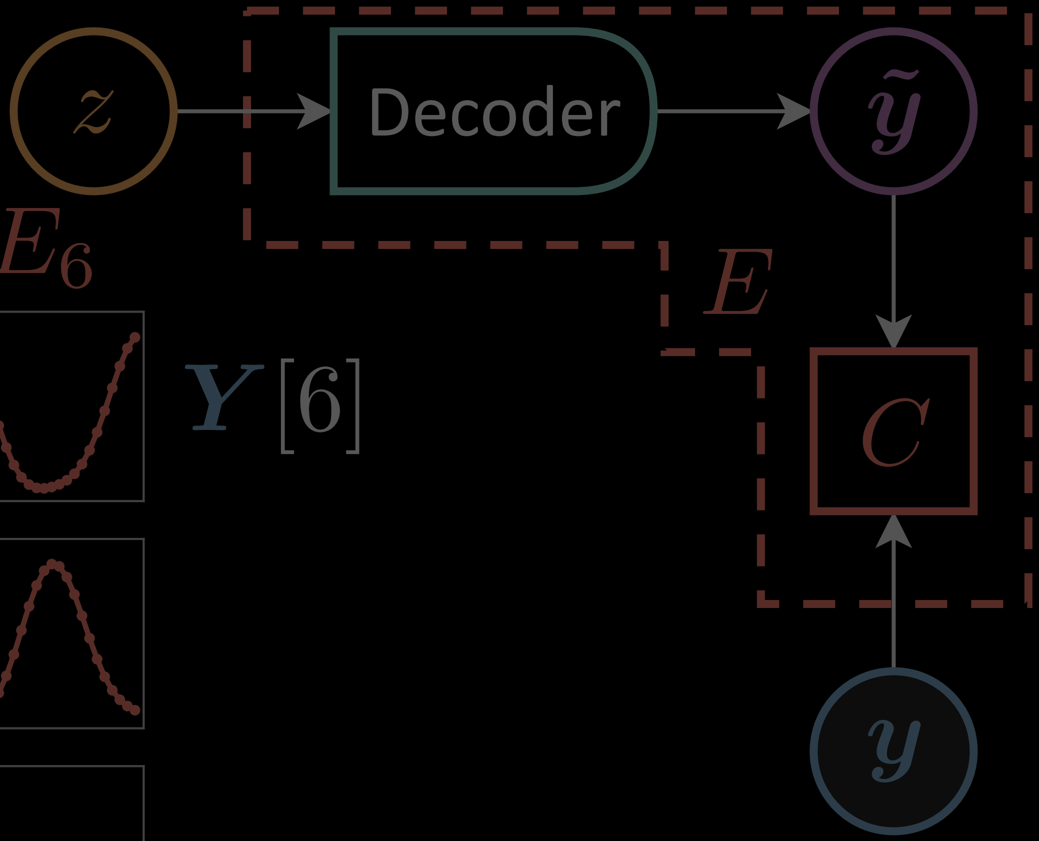




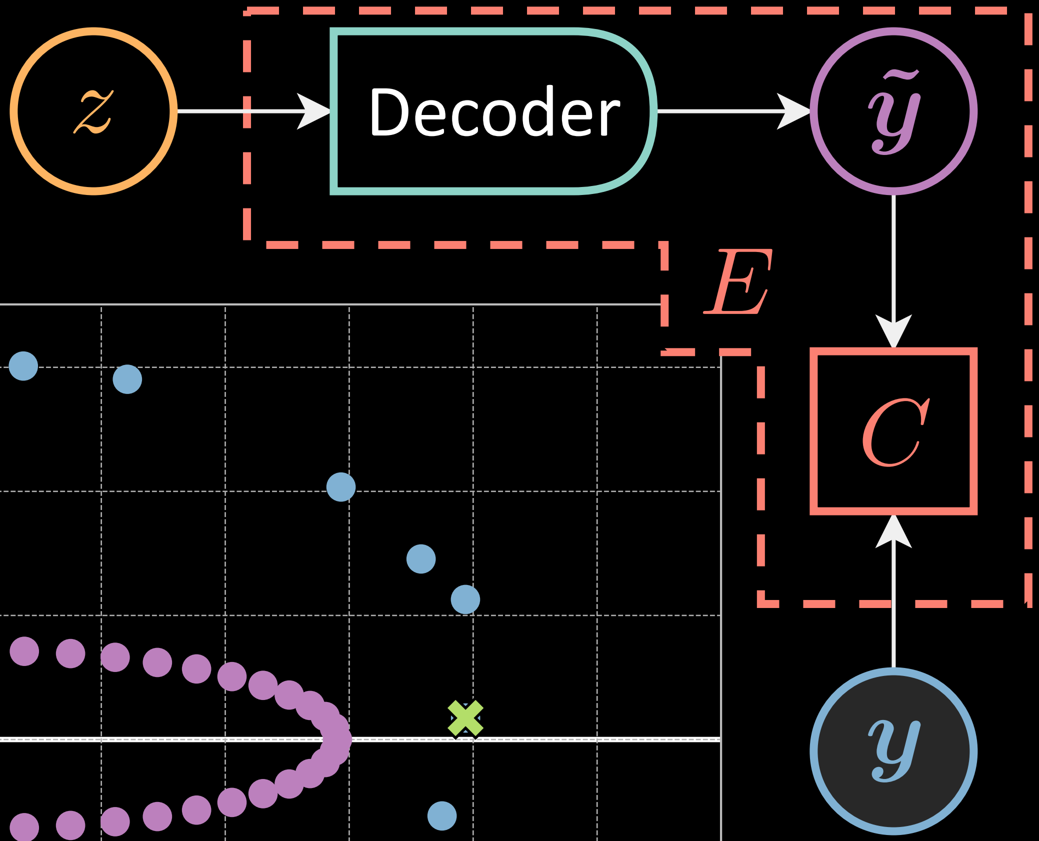
Energy function

$E(\boldsymbol{y}, z)$

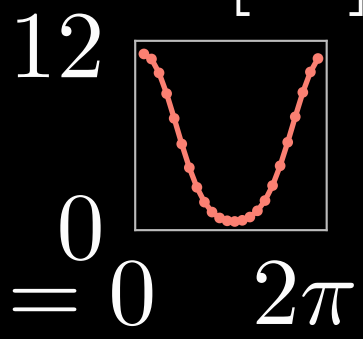


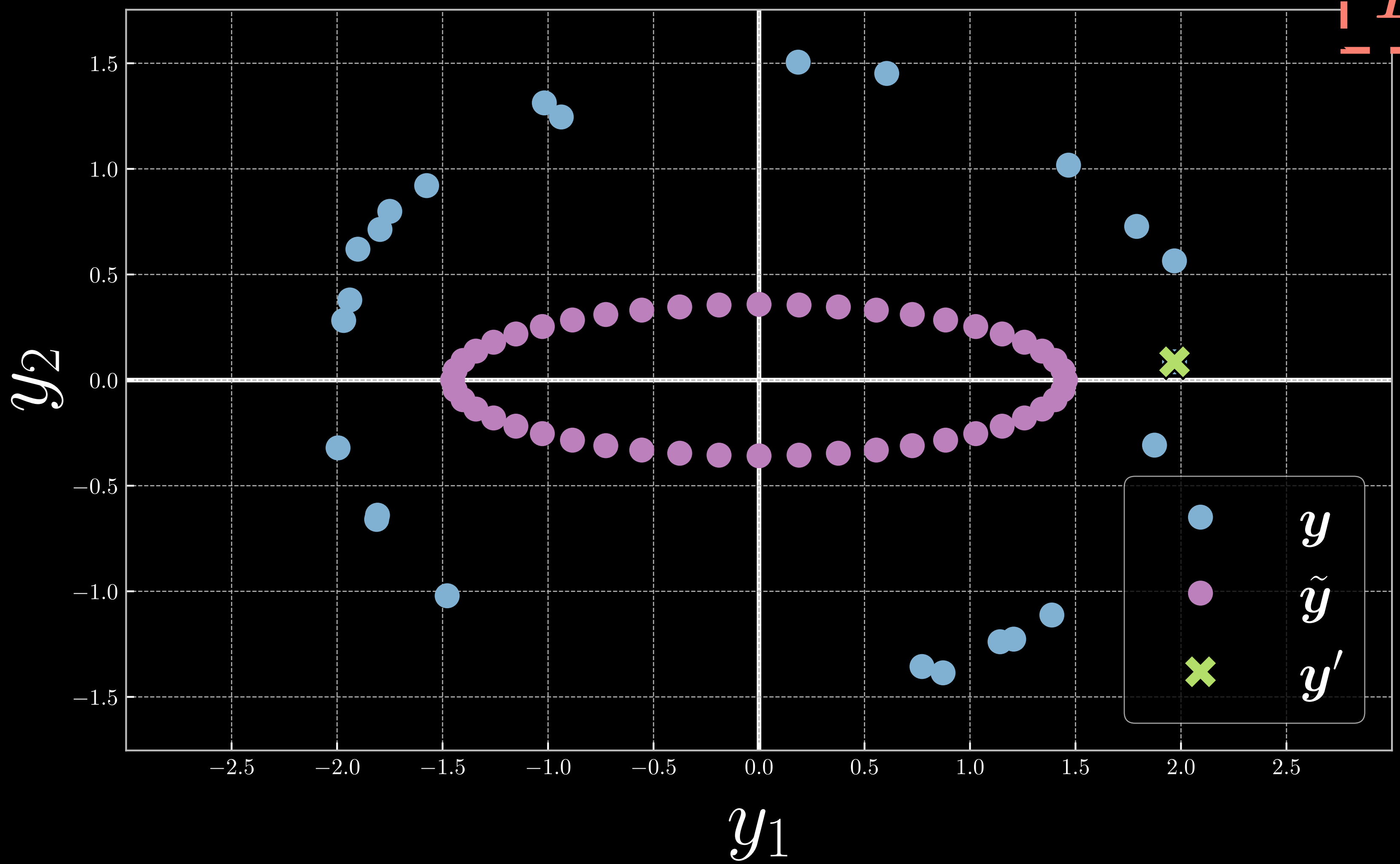


Energy function $E(y, z)$



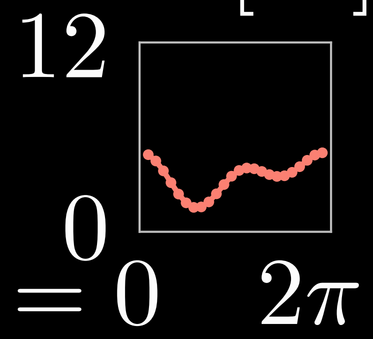
$y' = Y[23]$

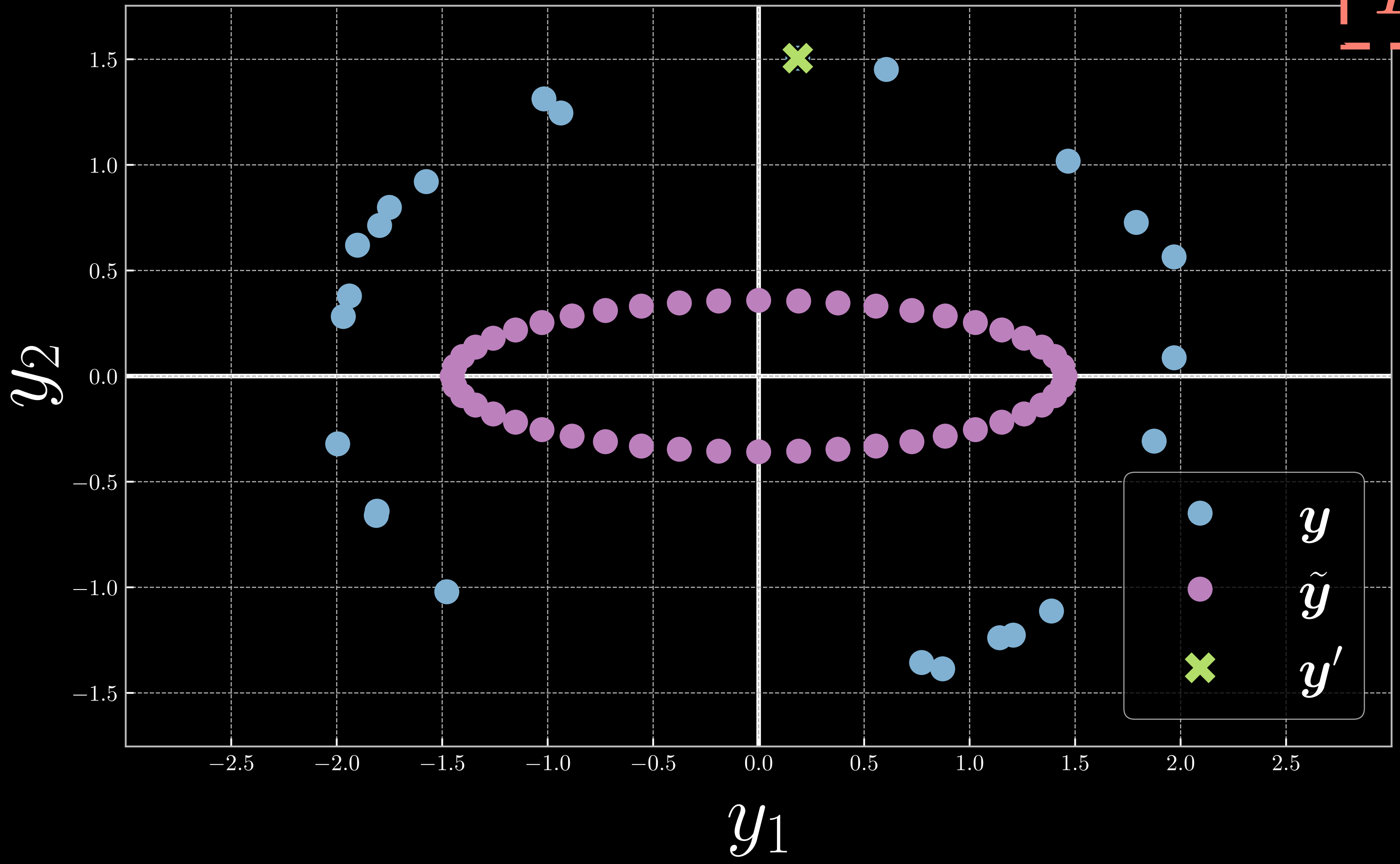


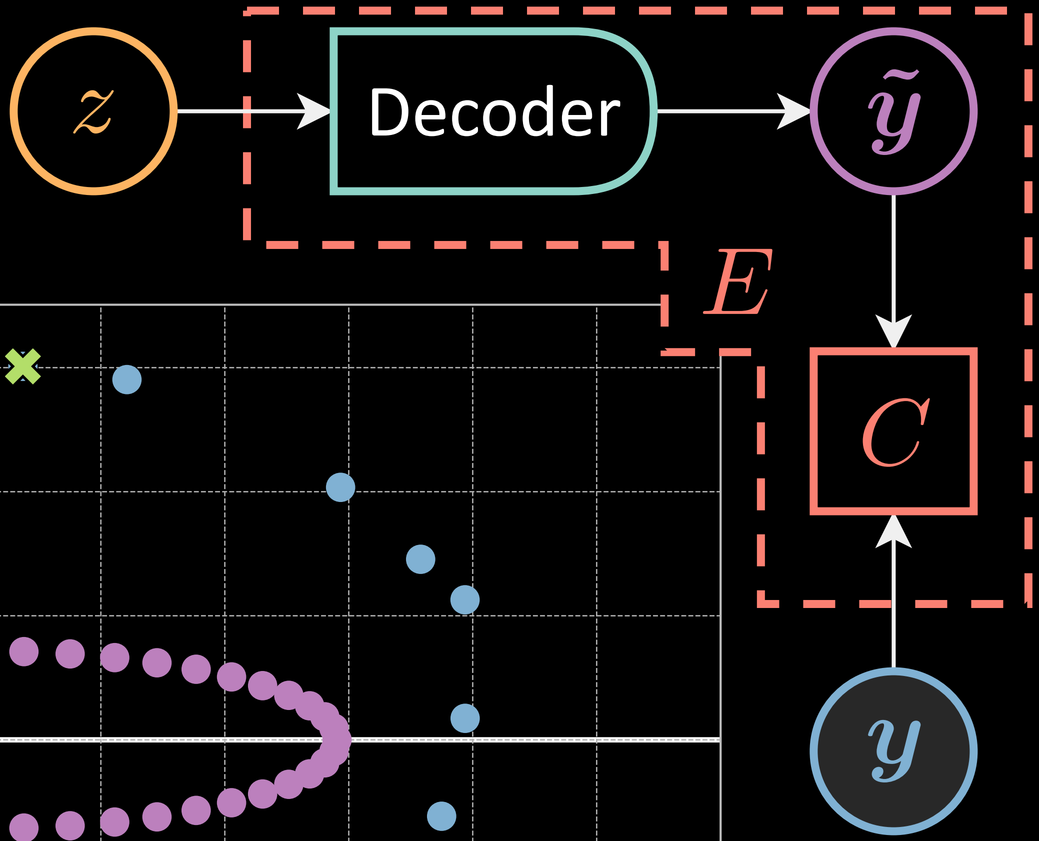


Energy function $E(\boldsymbol{y}, z)$

$\boldsymbol{y}' = \boldsymbol{Y}[10]$



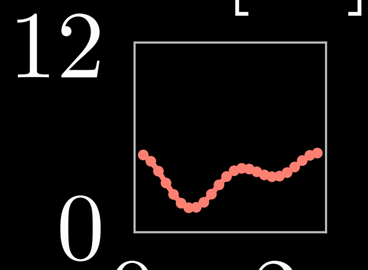




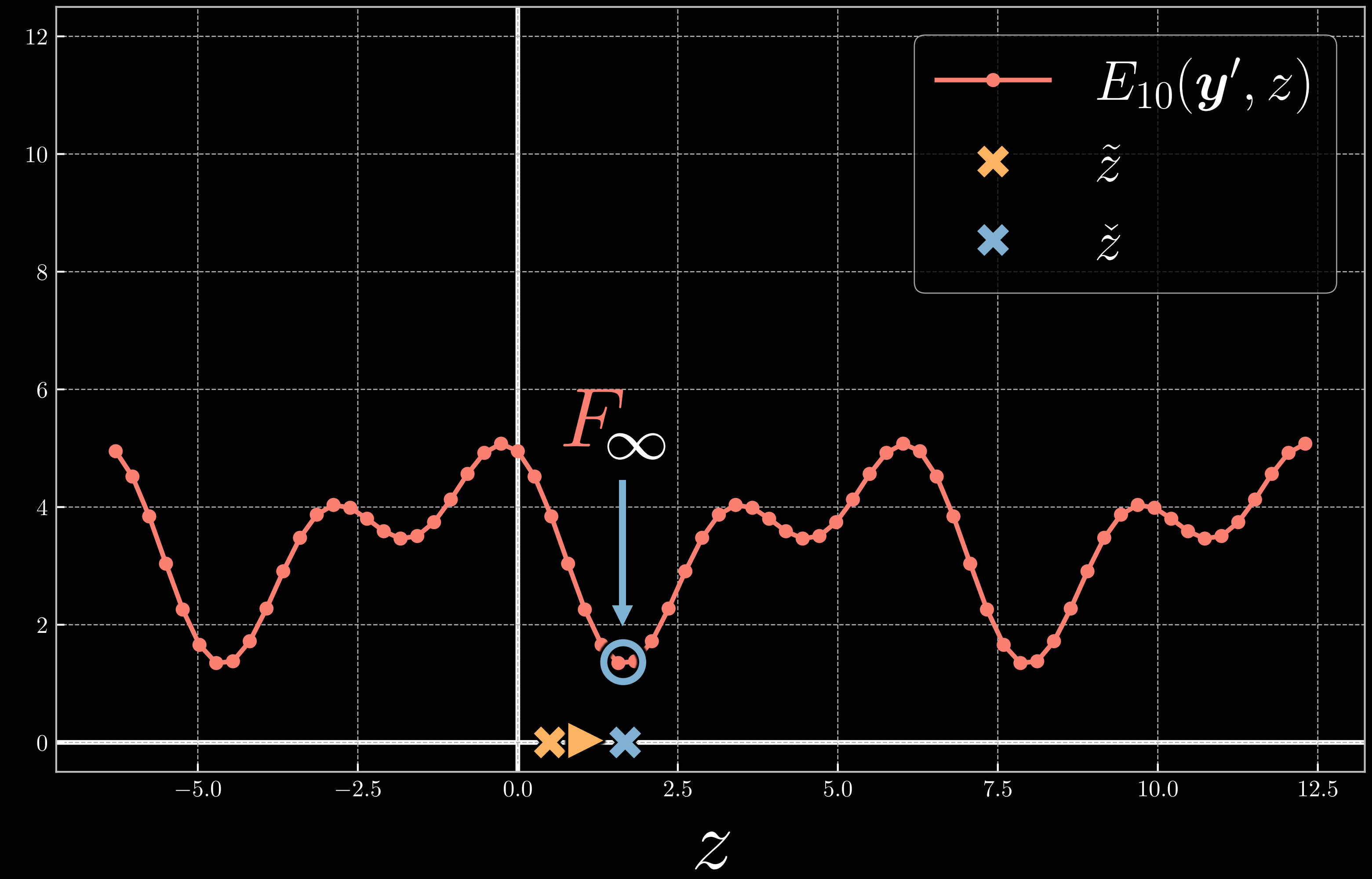
Free energy

$$F_\infty(\boldsymbol{y}) = \min_z E(\boldsymbol{y}, z) = E(\boldsymbol{y}, \check{z})$$

$$\boldsymbol{y}' = \boldsymbol{Y}[10]$$



$z = 0 \quad 2\pi$



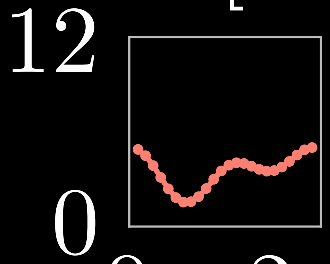
$$\check{z} = \arg\min_z E(\boldsymbol{y}, z)$$

exhaustive search, conjugate gradient, line search, LBFGS…

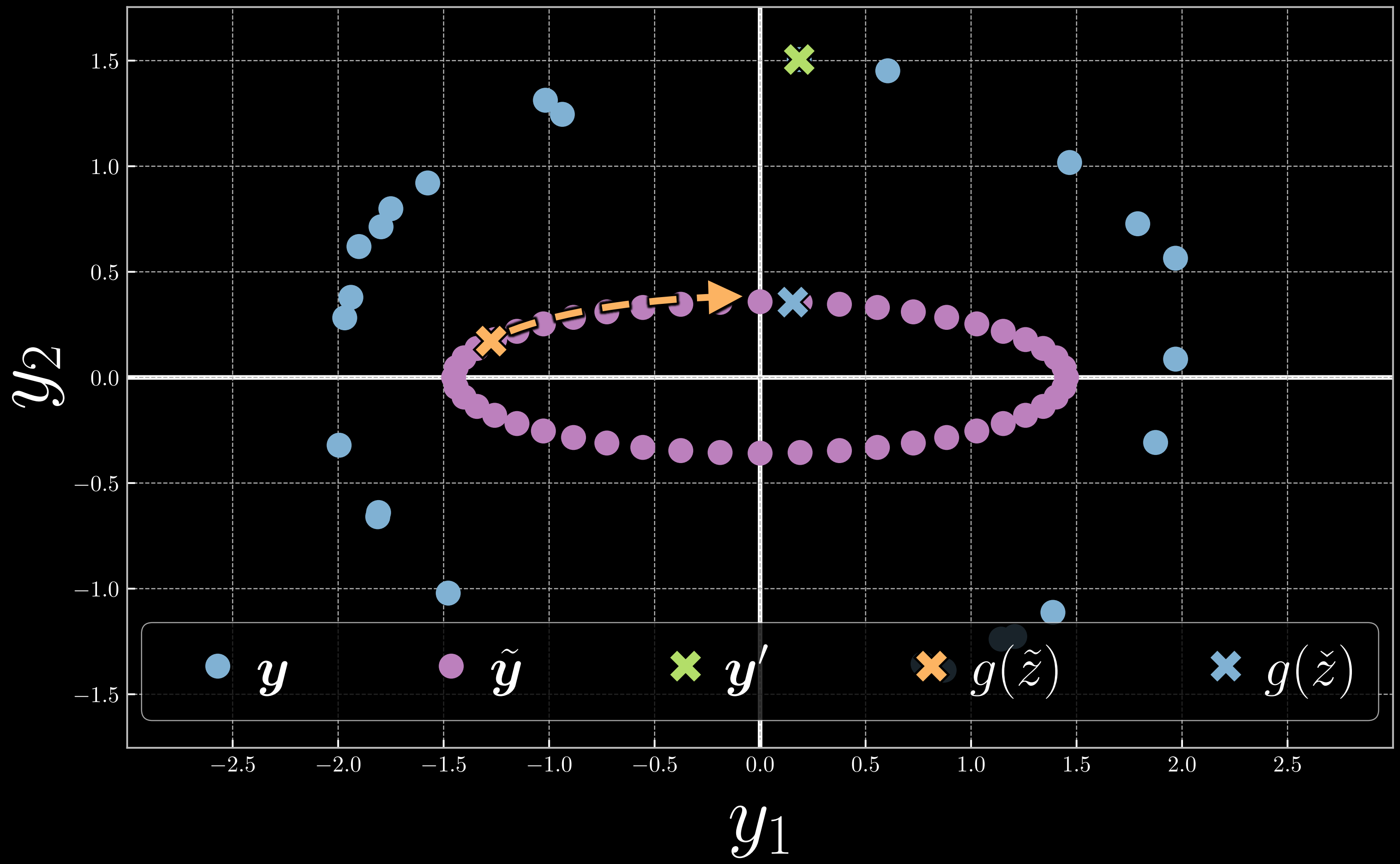
Free energy

$$F_\infty(\boldsymbol{y}) = \min_{z} E(\boldsymbol{y}, z) = E(\boldsymbol{y}, \check{z})$$

$$\boldsymbol{y}' = \boldsymbol{Y}[10]$$



$z = 0 \quad 2\pi$



$$\check{z} = \arg\min_{z} E(\boldsymbol{y}, z)$$

exhaustive search, conjugate gradient, line search, LBFGS…

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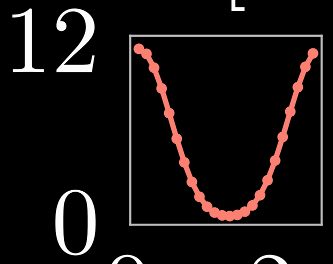

$$z = 0 \quad 2\pi$$

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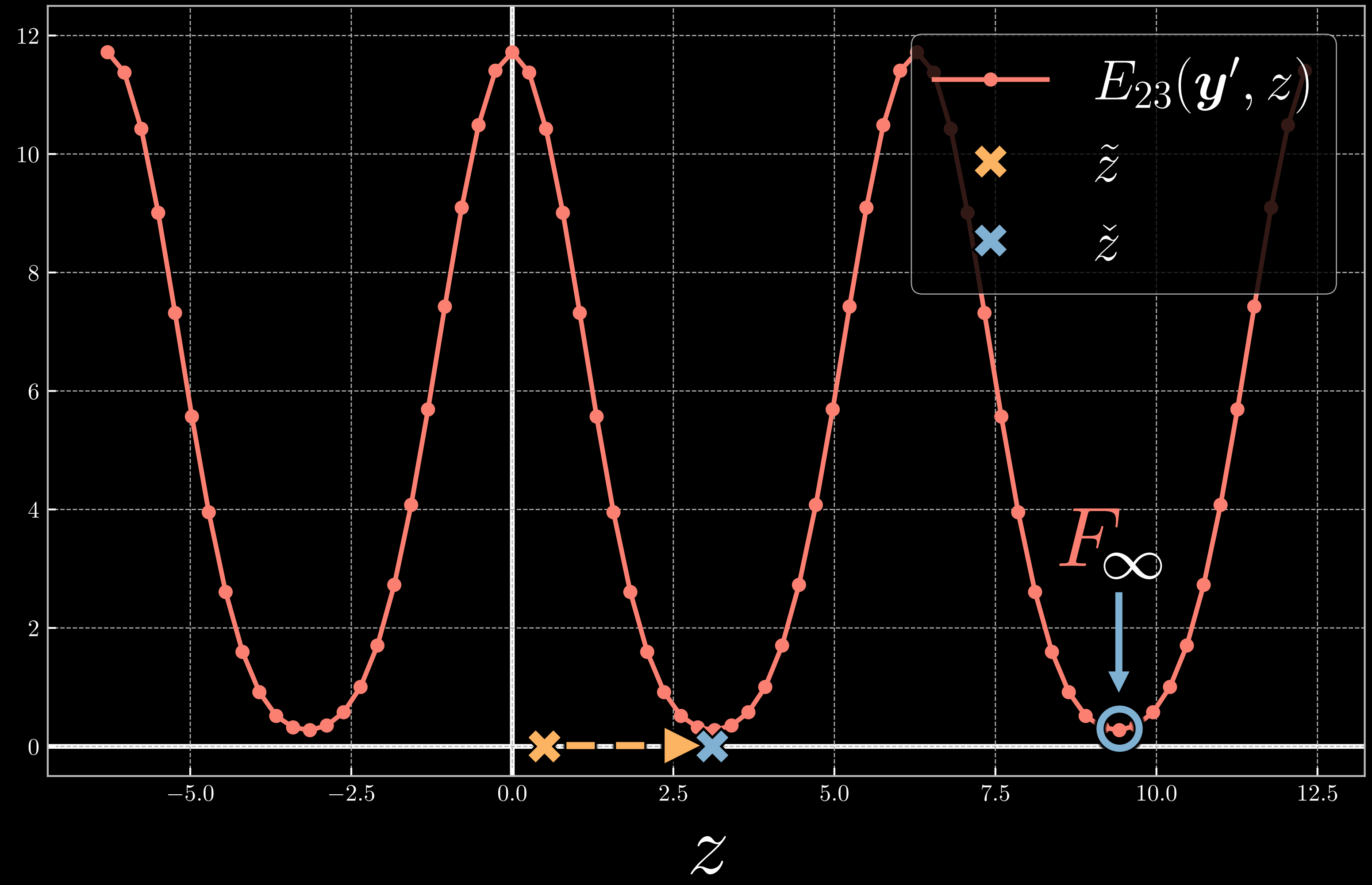

Free energy

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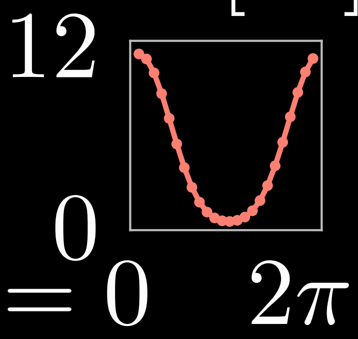

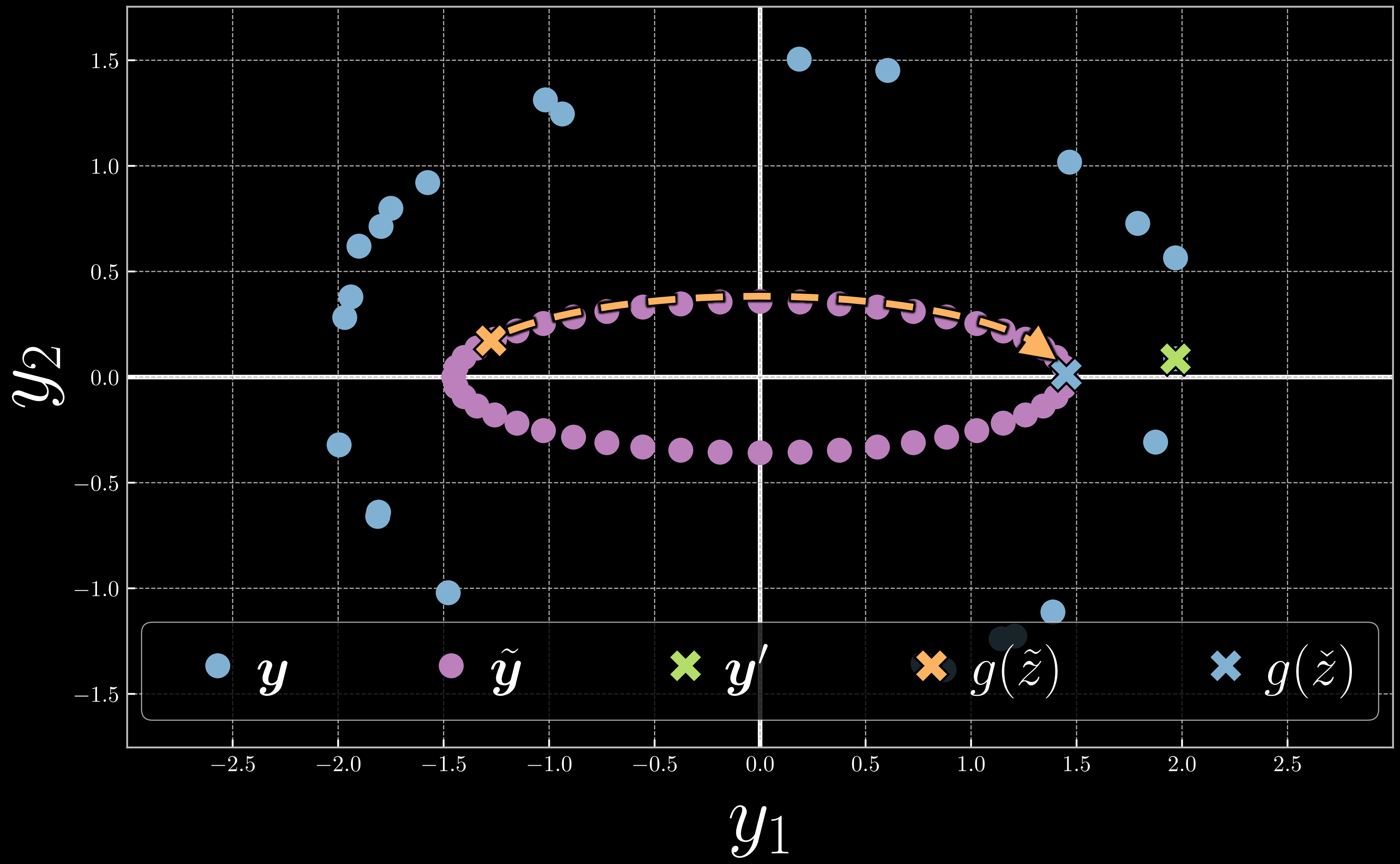

$$\check{z} = \arg\min_z E(\boldsymbol{y}, z)$$

exhaustive search, conjugate gradient, line search, LBFGS…

Free energy

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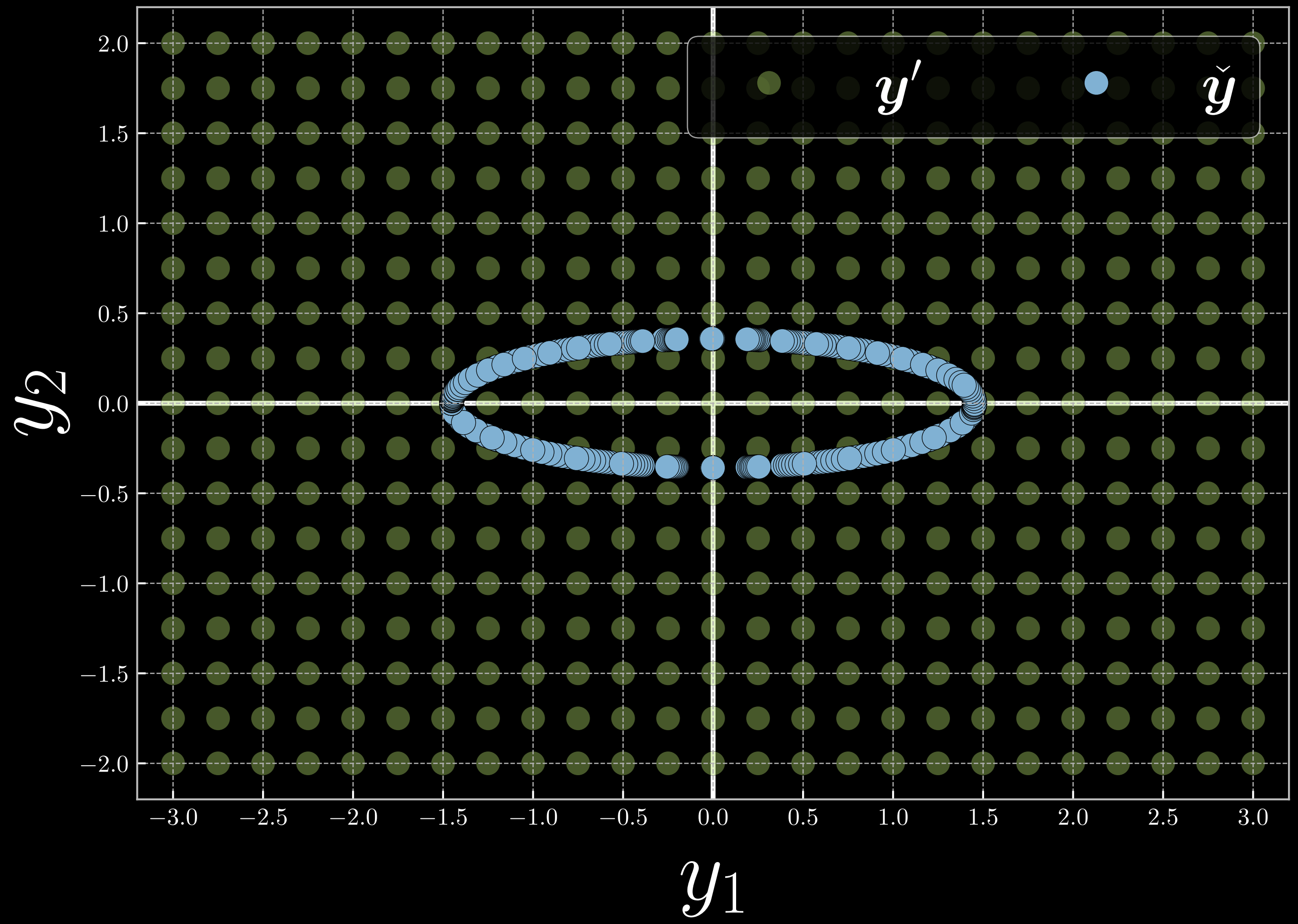

Free energy

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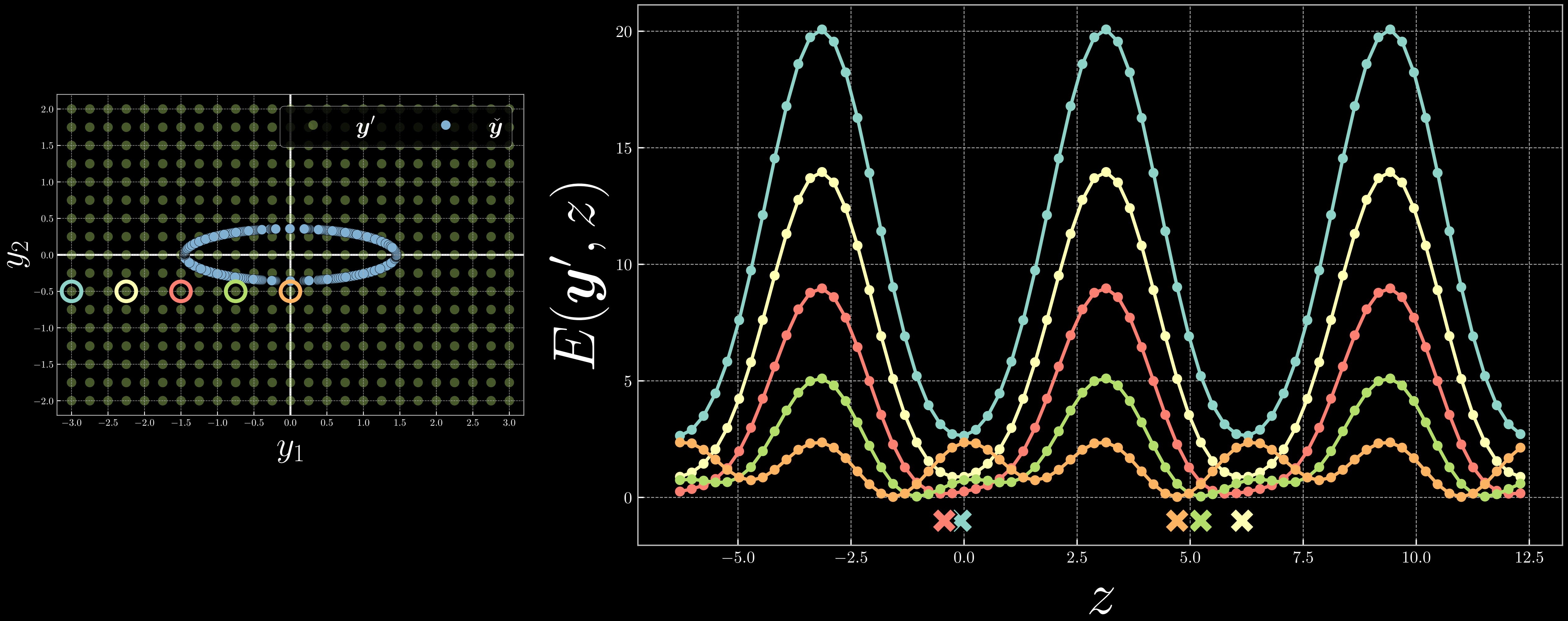

Free energy

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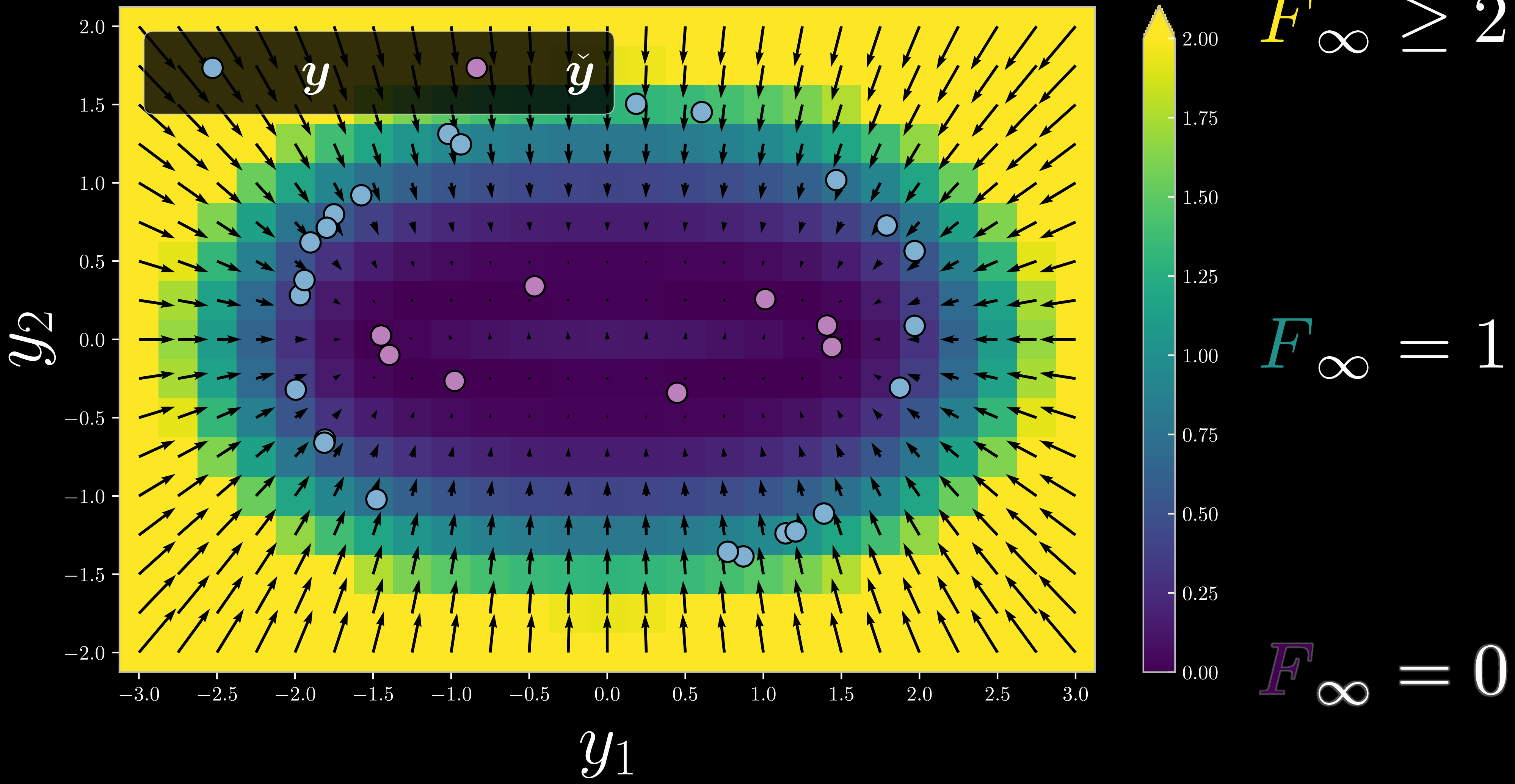

Free energy

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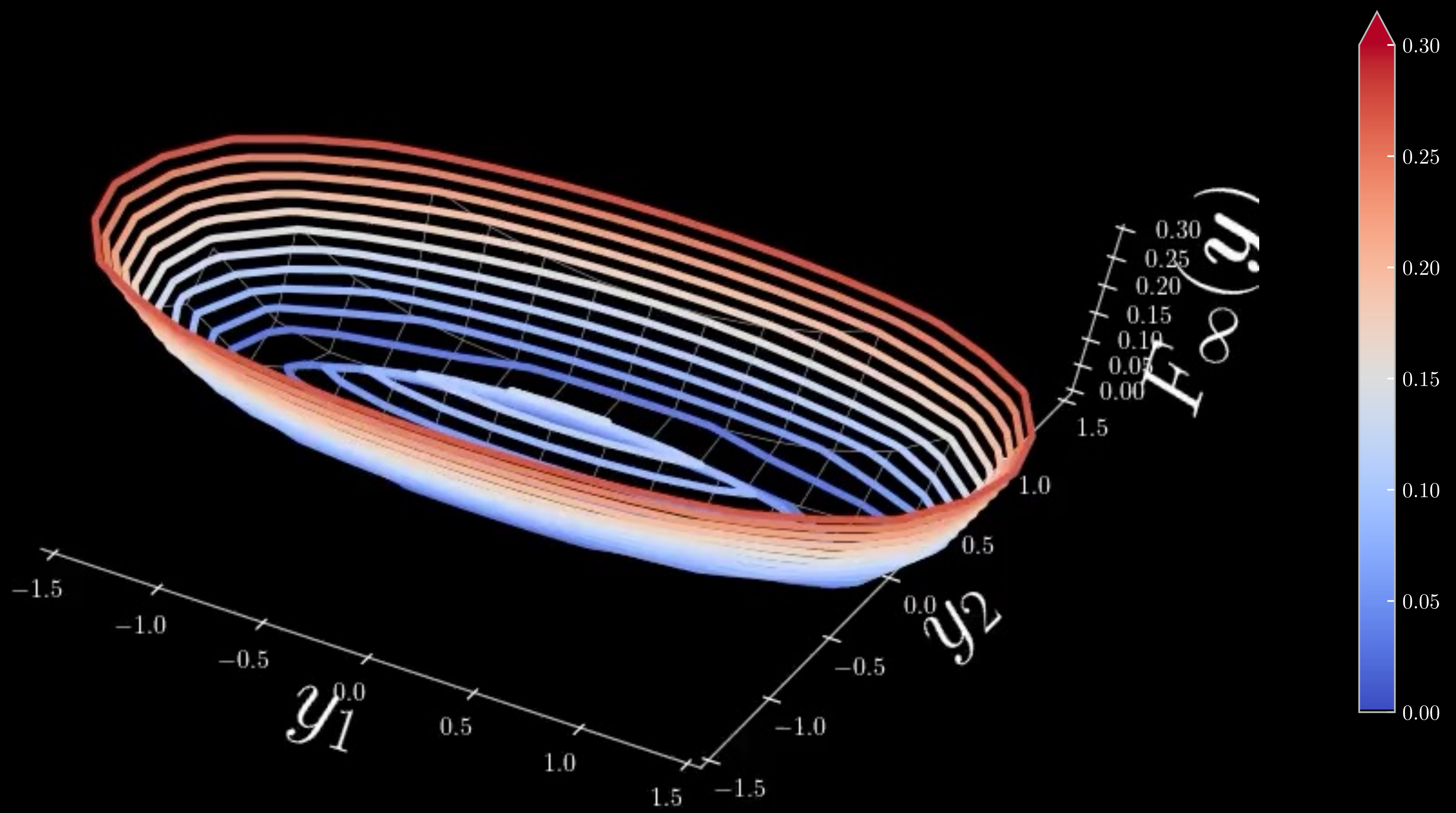


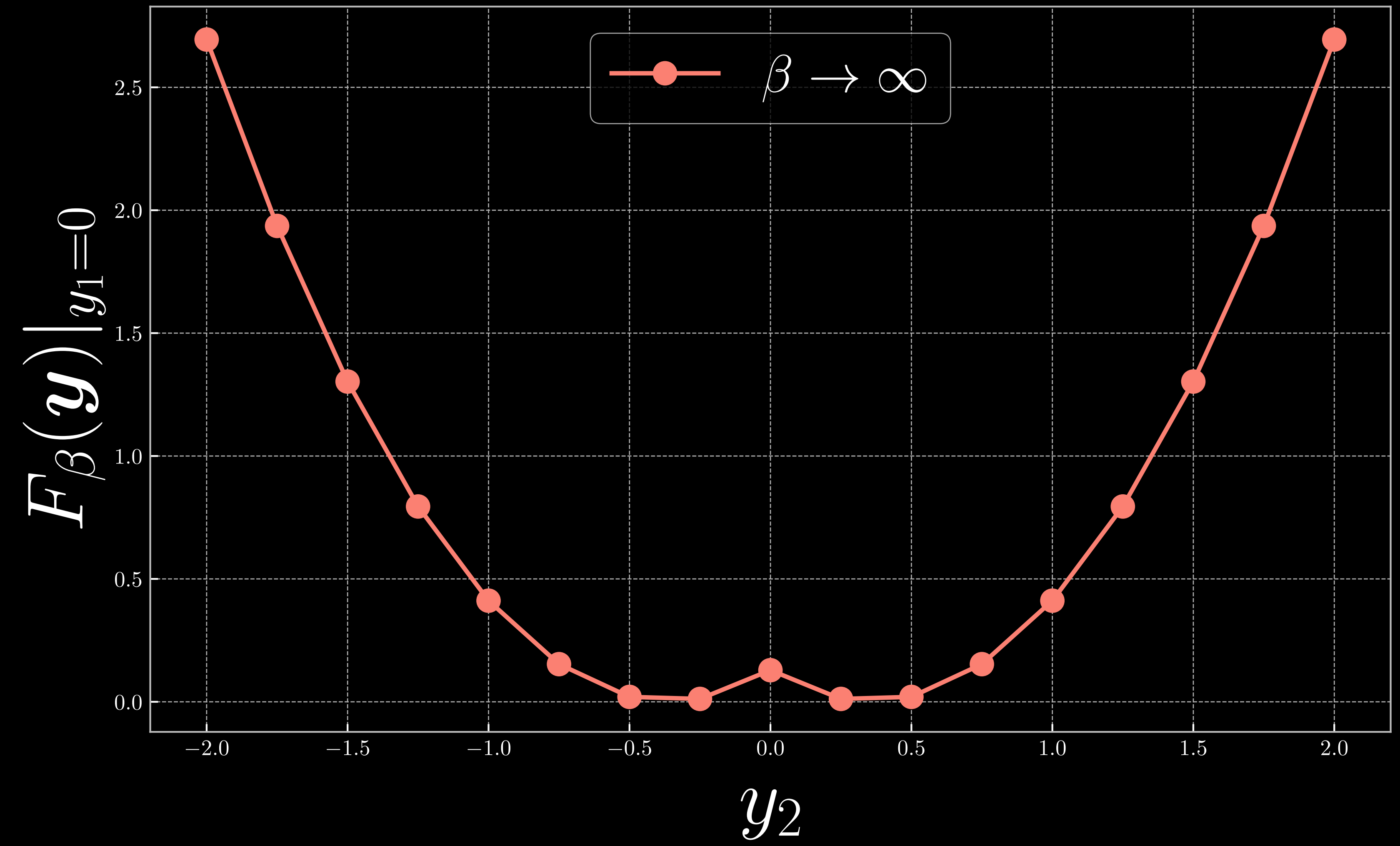
$F_\infty \geq 0.30$

$F_\infty = 0.15$

$F_\infty = 0.00$

Free energy

$$F_\infty(\boldsymbol{y}) = \min_z E(\boldsymbol{y}, z) = E(\boldsymbol{y}, \check{z})$$



Free energy

zero temperature limit free energy

$$F_\infty(\boldsymbol{y}) = \min_z E(\boldsymbol{y}, z) = E(\boldsymbol{y}, \check{z})$$

$$F_\beta(\boldsymbol{y}) \doteq -\frac{1}{\beta}\log\frac{1}{|\mathcal{Z}|}\int_{\mathcal{Z}} \exp[-\beta E(\boldsymbol{y}, z)]\,\mathrm{d}z$$

Boltzmann constant

average translational kinetic energy

$$\beta = (k_B T)^{-1}, \quad K_{\text{avg}} = \frac{3}{2}k_B T\ [\mathrm{J}]$$

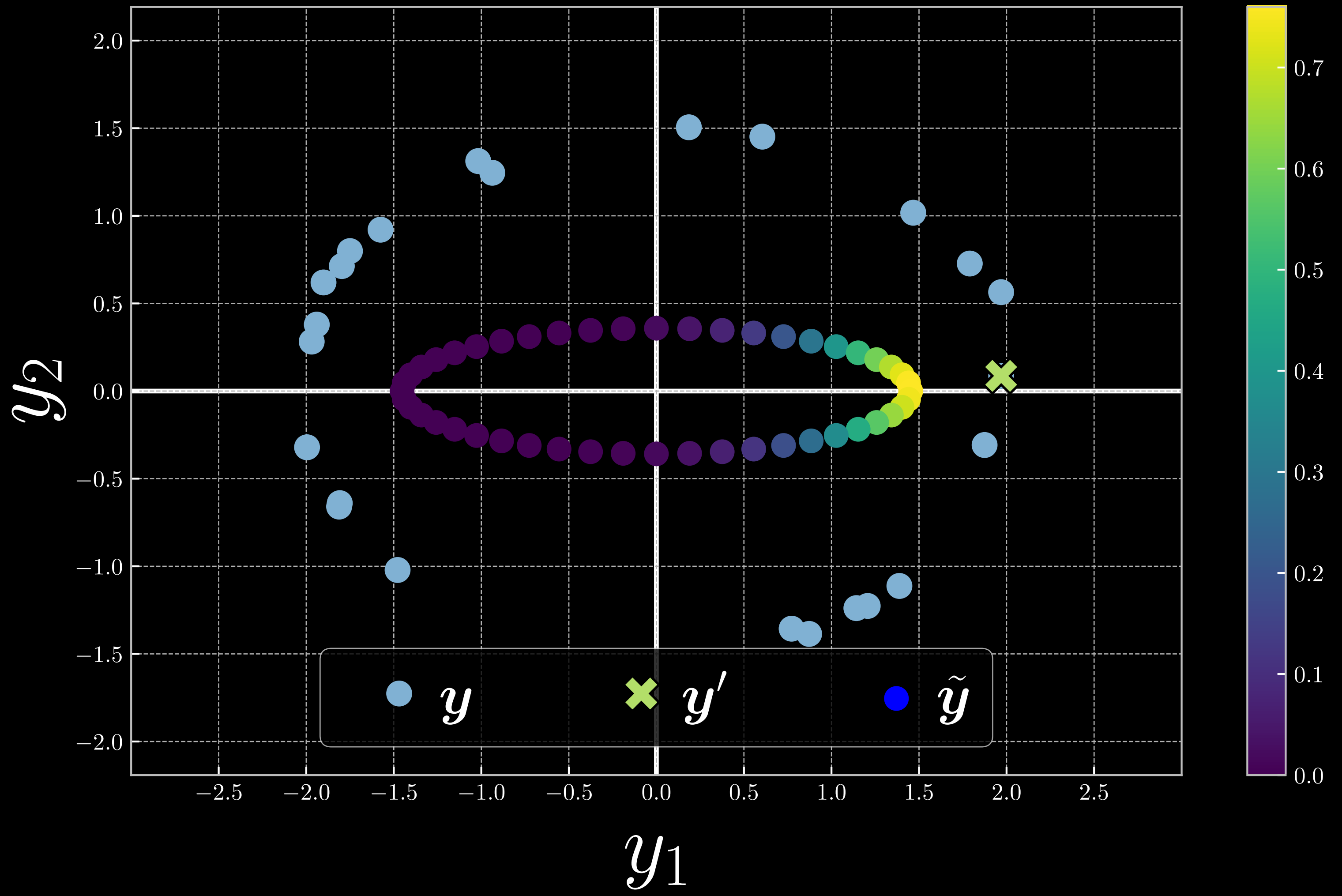
temperature

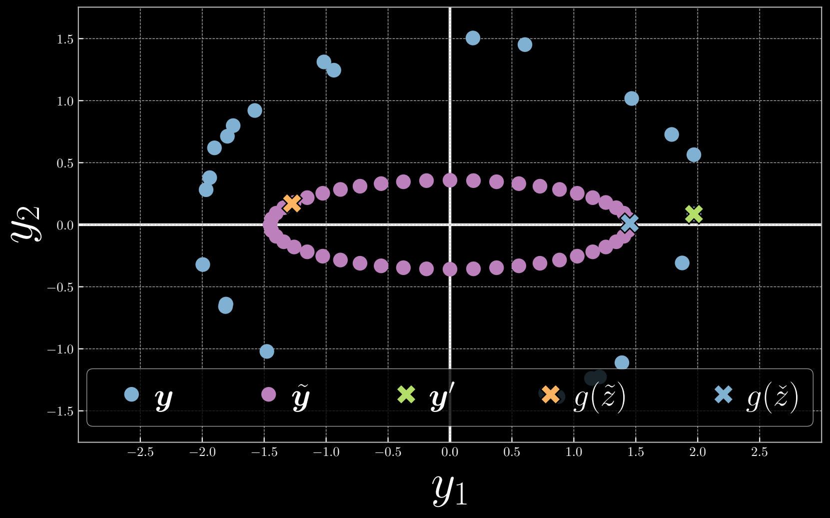
simple discrete approximation

$$\underbrace{\tilde{F}_\beta(\boldsymbol{y}) = -\frac{1}{\beta}\log\frac{1}{|\mathcal{Z}|}\sum_{z\in\mathcal{Z}} \exp[-\beta E(\boldsymbol{y}, z)]\,\Delta z}_{\operatorname{softmin}_\beta \langle E(\boldsymbol{y}, \mathcal{Z})\rangle}$$

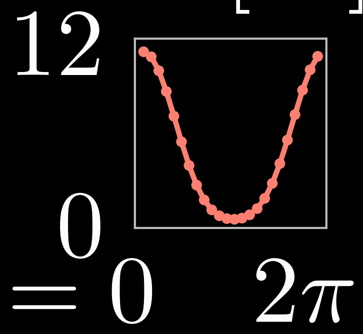
$$
\begin{aligned}
\lim_{\beta \to 0} F_\beta(\boldsymbol{y}) &= \lim_{\beta \to 0} -\frac{1}{\beta} \log \frac{1}{|\mathcal{Z}|} \int_{\mathcal{Z}} \exp[-\beta E(\boldsymbol{y}, z)] \, \mathrm{d}z = \\
&= \lim_{\beta \to 0} -\frac{\mathrm{d}}{\mathrm{d}\beta} \left[\log \frac{1}{|\mathcal{Z}|} + \log \int_{\mathcal{Z}} \exp[-\beta E(\boldsymbol{y}, z)] \, \mathrm{d}z \right] = \\
&= \lim_{\beta \to 0} -\frac{\mathrm{d}}{\mathrm{d}\beta} \log \int_{\mathcal{Z}} \exp[-\beta E(\boldsymbol{y}, z)] \, \mathrm{d}z = \\
&= \lim_{\beta \to 0} -\frac{1}{\int_{\mathcal{Z}} \exp[-\beta E(\boldsymbol{y}, z)] \, \mathrm{d}z} \frac{\mathrm{d}}{\mathrm{d}\beta} \int_{\mathcal{Z}} \exp[-\beta E(\boldsymbol{y}, z)] \, \mathrm{d}z = \\
&= \lim_{\beta \to 0} -\frac{1}{\int_{\mathcal{Z}} \exp[-\beta E(\boldsymbol{y}, z)] \, \mathrm{d}z} \int_{\mathcal{Z}} -E(\boldsymbol{y}, z) \exp[-\beta E(\boldsymbol{y}, z)] \, \mathrm{d}z = \\
&= \frac{1}{|\mathcal{Z}|} \int_{\mathcal{Z}} E(\boldsymbol{y}, z) \, \mathrm{d}z = \langle E(\boldsymbol{y}, z) \rangle
\end{aligned}
$$

Free energy $F_\beta(\boldsymbol{y}) \doteq -\frac{1}{\beta} \log \frac{1}{|\mathcal{Z}|} \int_{\mathcal{Z}} \exp[-\beta E(\boldsymbol{y}, z)] \, \mathrm{d}z$



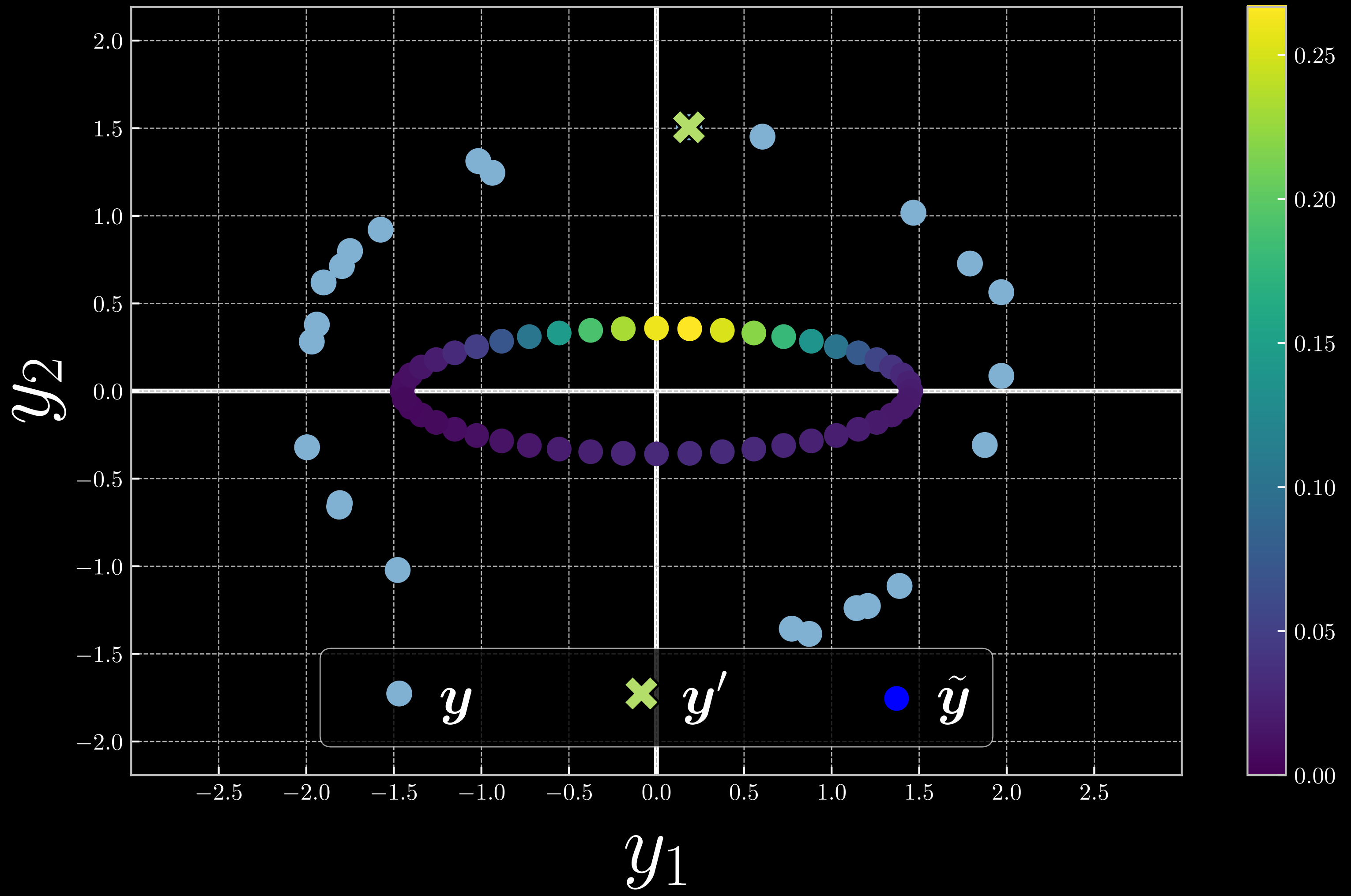


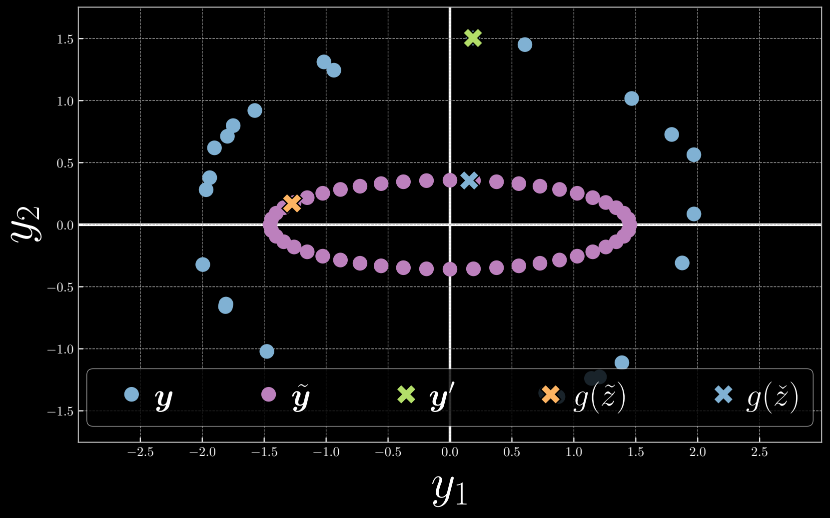
$\boldsymbol{y}' = \boldsymbol{Y}[23]$



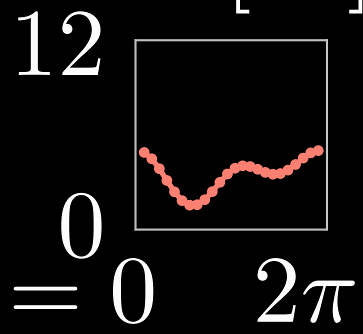
$\beta = 1$

Free energy $F_\beta(\boldsymbol{y}) \doteq -\frac{1}{\beta} \log \frac{1}{|\mathcal{Z}|} \int_{\mathcal{Z}} \exp[-\beta E(\boldsymbol{y}, z)]\, \mathrm{d}z$



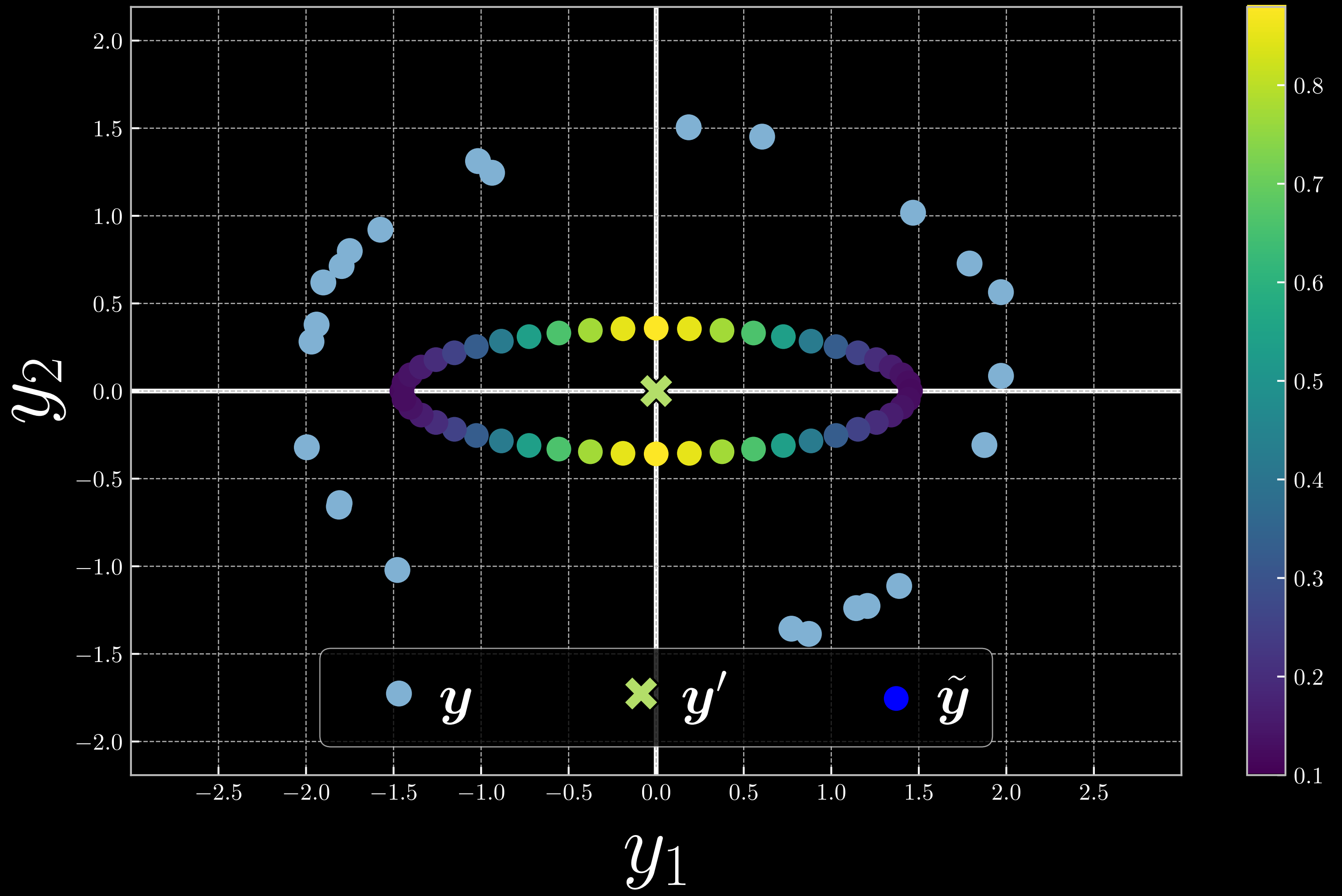


$\boldsymbol{y}' = \boldsymbol{Y}[10]$



$\beta = 1$

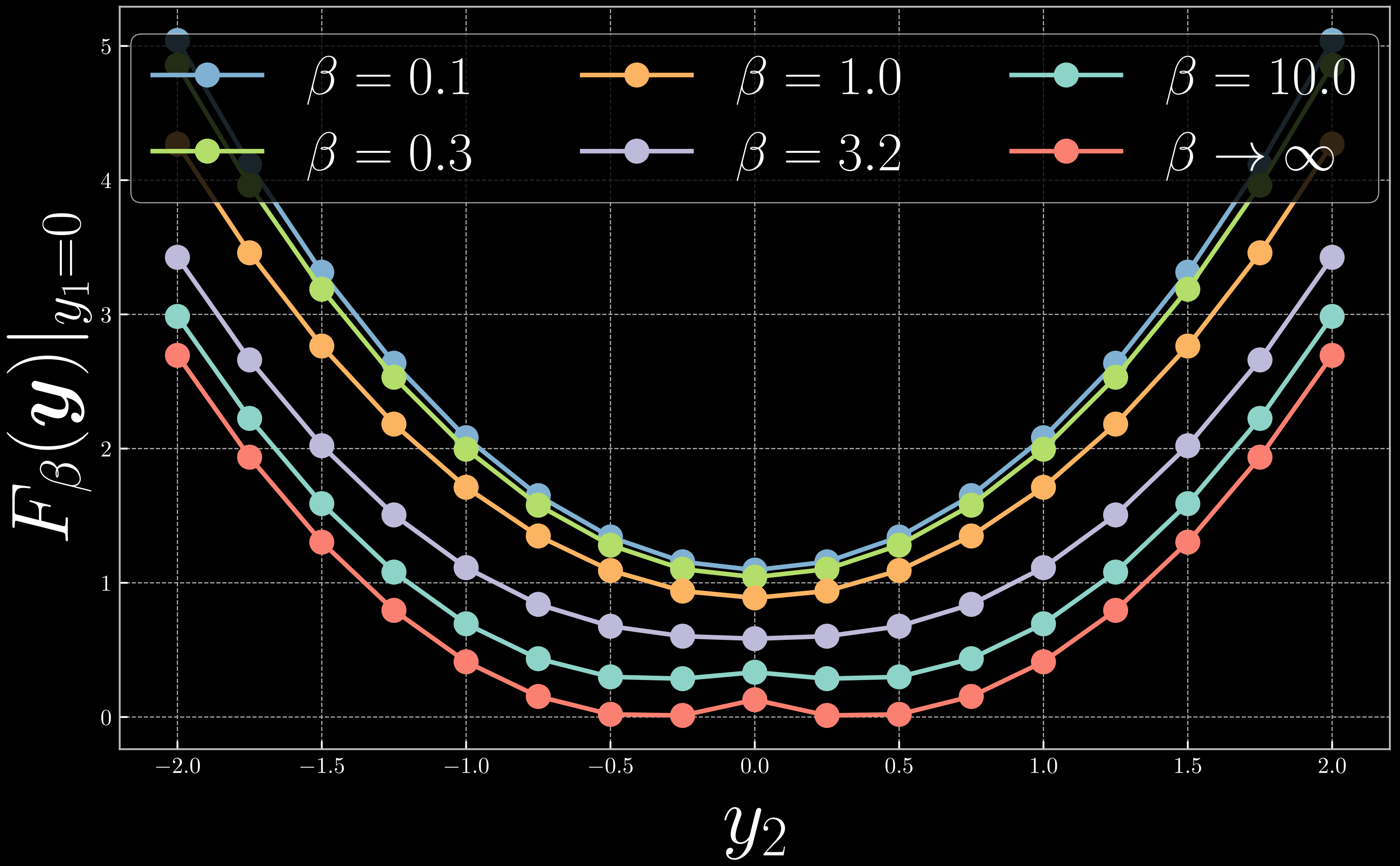
Free energy $F_\beta(\boldsymbol{y}) \doteq -\frac{1}{\beta}\log\frac{1}{|\mathcal{Z}|}\int_{\mathcal{Z}}\exp[-\beta E(\boldsymbol{y}, z)]\,\mathrm{d}z$



$\boldsymbol{y}' = (0, 0)$

$\beta = 1$

Free energy $F_\beta(\boldsymbol{y}) \doteq -\frac{1}{\beta}\log\frac{1}{|\mathcal{Z}|}\int_{\mathcal{Z}}\exp[-\beta E(\boldsymbol{y}, z)]\,\mathrm{d}z$



Nomenclature and PyTorch

$$\frac{|\mathcal{Z}|}{\Delta z}$$

$$\text{softmax}_\beta \langle E(\boldsymbol{y}, \mathcal{Z}) \rangle \doteq \frac{1}{\beta} \log \sum_{z \in \mathcal{Z}} \exp[\beta E(\boldsymbol{y}, z)] - \underbrace{\frac{1}{\beta} \log N_z}$$

$$= \frac{1}{\beta} \texttt{torch.logsumexp(}\beta E(\boldsymbol{y}, z)\texttt{, dim=}z\texttt{)}$$

average softmin

$$\text{softmin}_\beta \langle E(\boldsymbol{y}, \mathcal{Z}) \rangle \doteq -\frac{1}{\beta} \log \frac{1}{N_z} \sum_{z \in \mathcal{Z}} \exp[-\beta E(\boldsymbol{y}, z)]$$

$$= -\text{softmax}_\beta \langle -E(\boldsymbol{y}, \mathcal{Z}) \rangle$$

$$\texttt{torch.softmax(}\mathbf{s}\texttt{)} = \text{softargmax}_{\beta=1}(\mathbf{s})$$

TRAINING

Finding a well behaved energy function

previously... loss function

$\mathcal{L}(\boldsymbol{w}, \mathcal{S}) \in \mathbb{R}$

Loss functional

$$\mathcal{L}[F(\mathcal{Y}), \boldsymbol{Y}] \doteq \frac{1}{P} \sum_{p=1}^{P} L[F(\mathcal{Y}), \boldsymbol{y}^{(p)}] \in \mathbb{R}$$

$$L_{\text{energy}}[F(\mathcal{Y}), \boldsymbol{y}] = F(\boldsymbol{y})$$

$$L_{\text{hinge}}[F(\mathcal{Y}), \boldsymbol{y}, \hat{\boldsymbol{y}}] = (m - [F(\hat{\boldsymbol{y}}) - F(\boldsymbol{y})])^{+}$$

$$L_{\log}[F(\mathcal{Y}), \boldsymbol{y}, \hat{\boldsymbol{y}}] = \log(1 + \exp[F(\boldsymbol{y}) - F(\hat{\boldsymbol{y}})])$$

$$= \text{softplus}[F(\boldsymbol{y}) - F(\hat{\boldsymbol{y}})]$$

previously… loss function

$$\mathcal{L}(\boldsymbol{w}, \mathcal{S}) \in \mathbb{R}$$

Loss functional

$$\mathcal{L}[F(\mathcal{Y}), \boldsymbol{Y}] \doteq \frac{1}{P} \sum_{p=1}^{P} L[F(\mathcal{Y}), \boldsymbol{y}^{(p)}] \in \mathbb{R}$$

$$L_{\text{energy}}[F(\mathcal{Y}), \boldsymbol{y}] = F(\boldsymbol{y})$$

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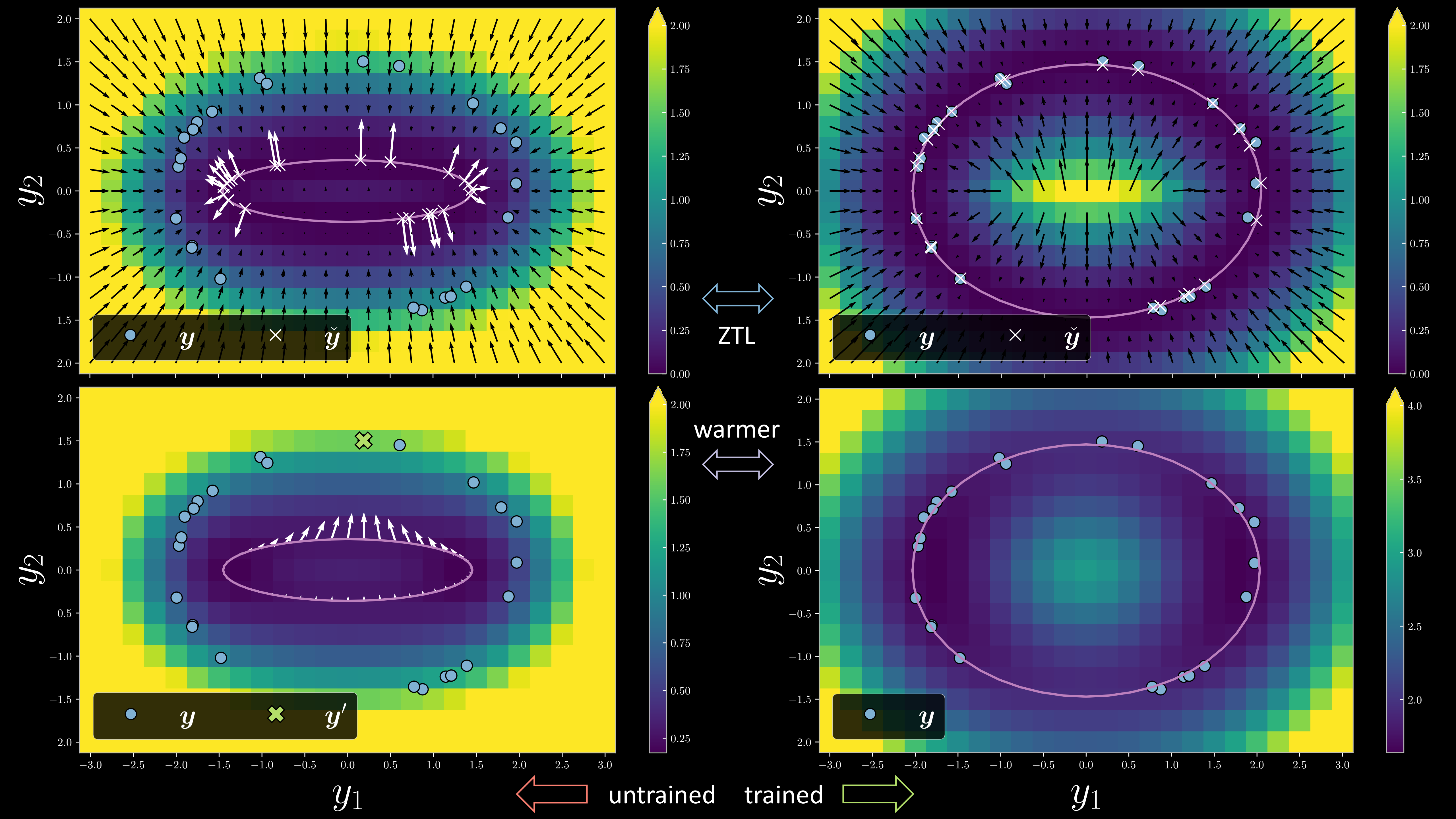
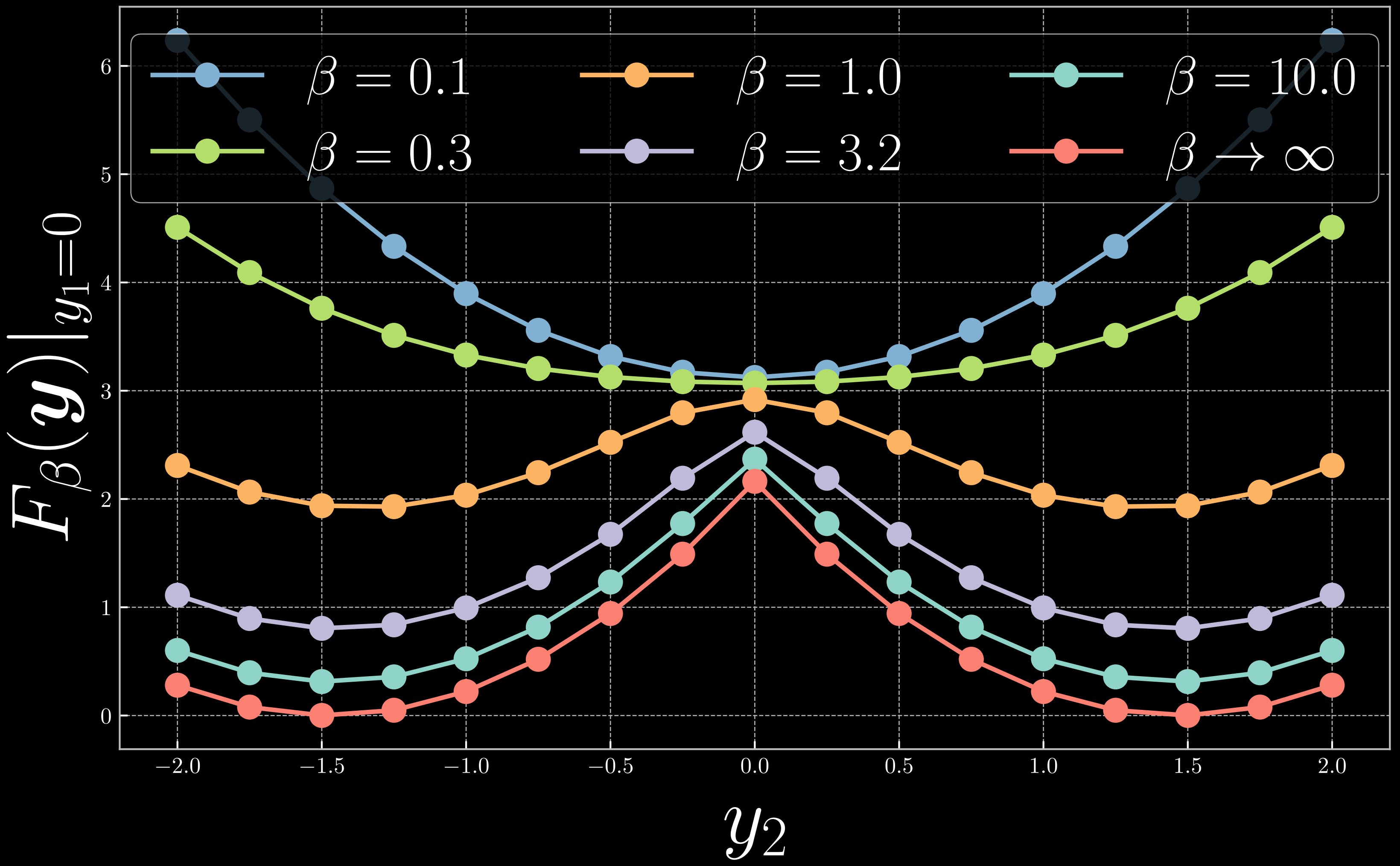
$$L_{\log}[F(\mathcal{Y}), \boldsymbol{y}, \hat{\boldsymbol{y}}] = \log(1 + \exp[F(\boldsymbol{y}) - F(\hat{\boldsymbol{y}})])$$

$$= \text{softplus}[F(\boldsymbol{y}) - F(\hat{\boldsymbol{y}})]$$



ZTL
warmer
untrained
trained
y
$\check{y}$
y'
y_1
y_2

Free energy $F_\beta(\boldsymbol{y}) \doteq -\frac{1}{\beta} \log \frac{1}{|\mathcal{Z}|} \int_{\mathcal{Z}} \exp[-\beta E(\boldsymbol{y}, z)] \, \mathrm{d}z$



Self-supervised learning

Conditional case

Training samples

$$\alpha = 1.5$$
$$\beta = 2$$

$$\boldsymbol{y} = \begin{bmatrix} \rho_1(x)\cos(\theta) + \varepsilon \\ \rho_2(x)\sin(\theta) + \varepsilon \end{bmatrix}$$

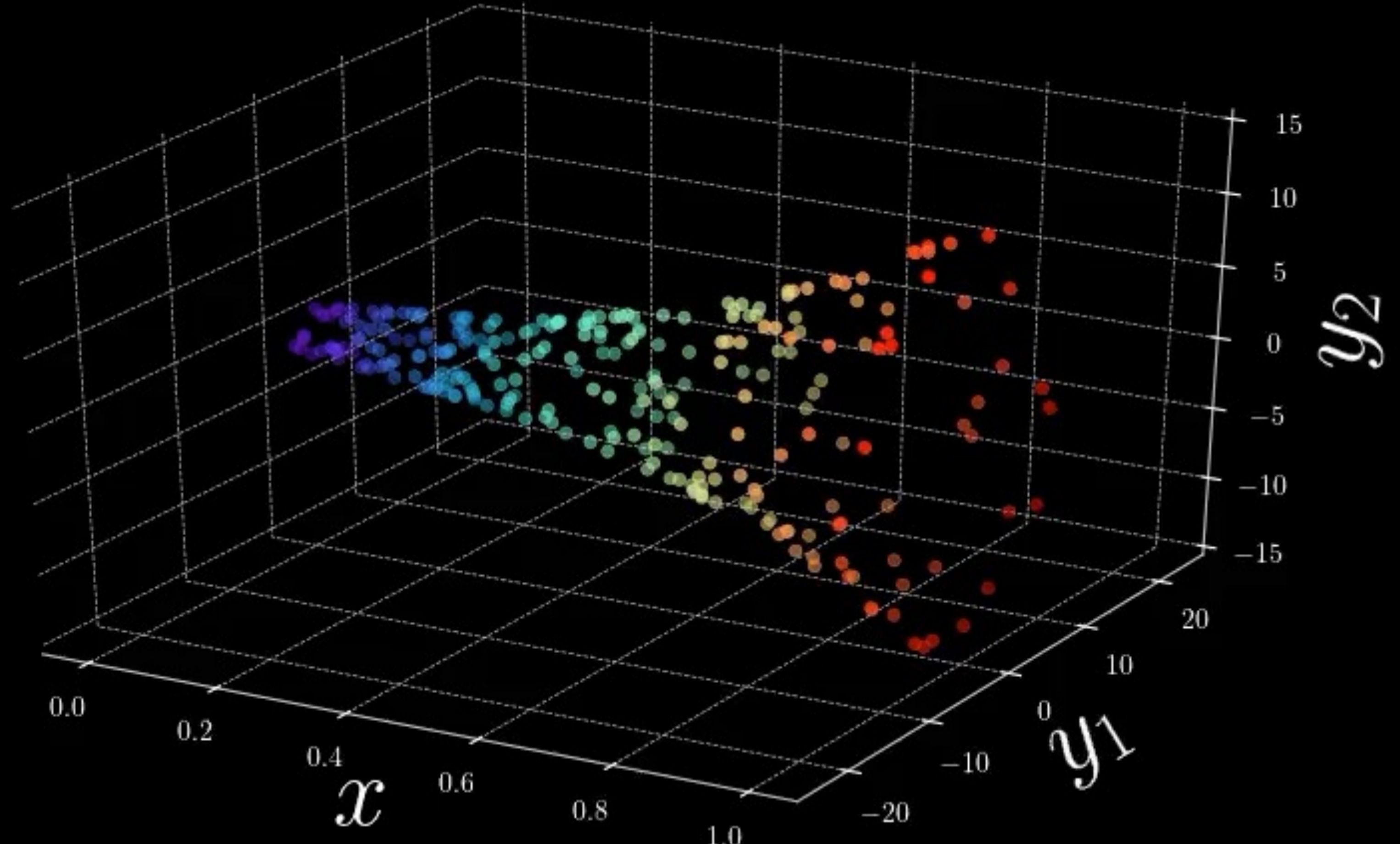
$$\rho : \mathbb{R} \to \mathbb{R}^2$$

$$x \mapsto \begin{bmatrix} \alpha x + \beta(1-x) \\ \beta x + \alpha(1-x) \end{bmatrix} \cdot \exp(2x)$$

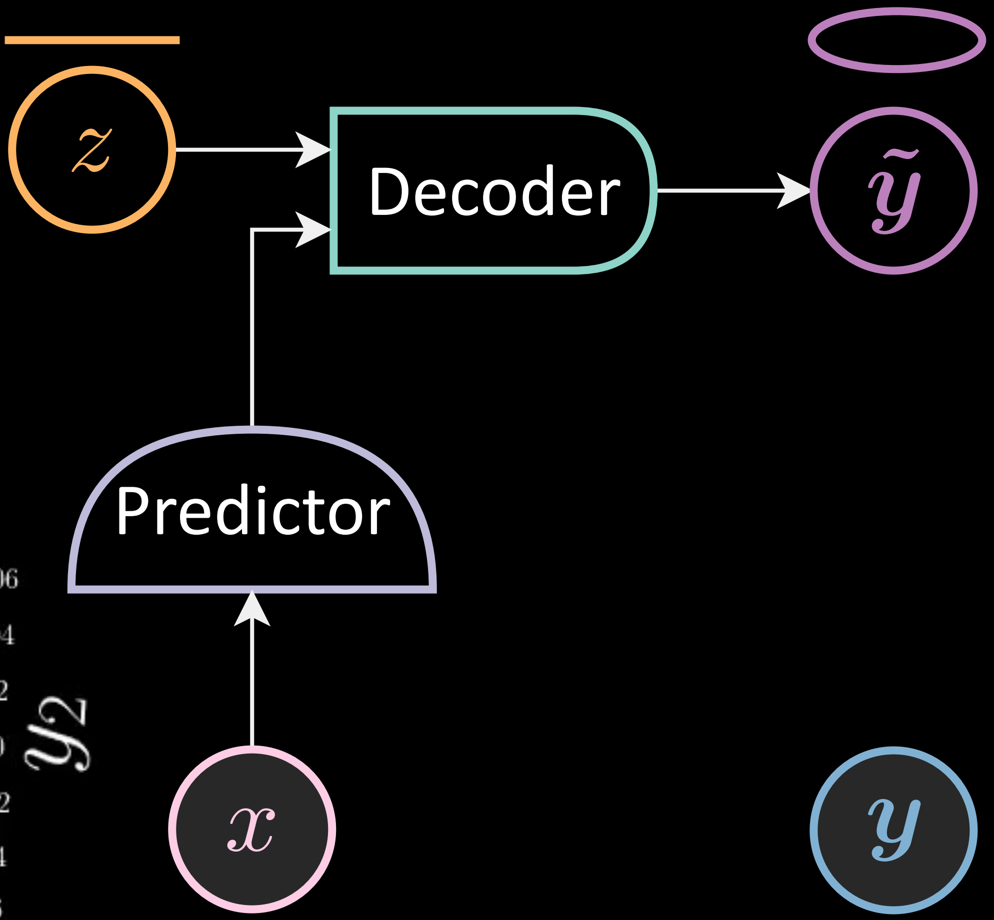
$$x \sim \mathcal{U}(0,1)$$

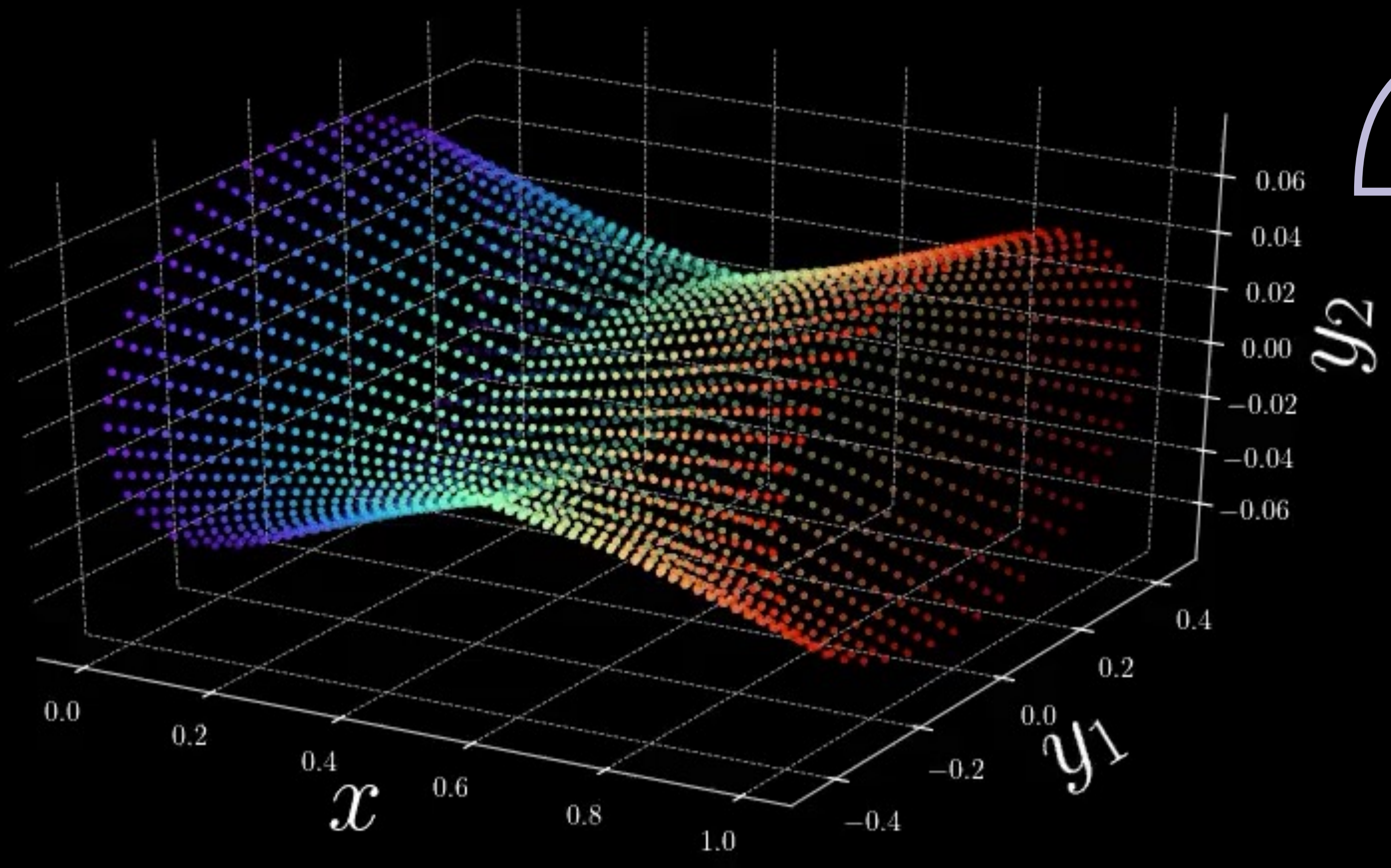
$$\theta \sim \mathcal{U}(0,2\pi)$$

$$\varepsilon \sim \mathcal{N}\left[0, \left(\tfrac{1}{20}\right)^2\right]$$



Untrained model manifold

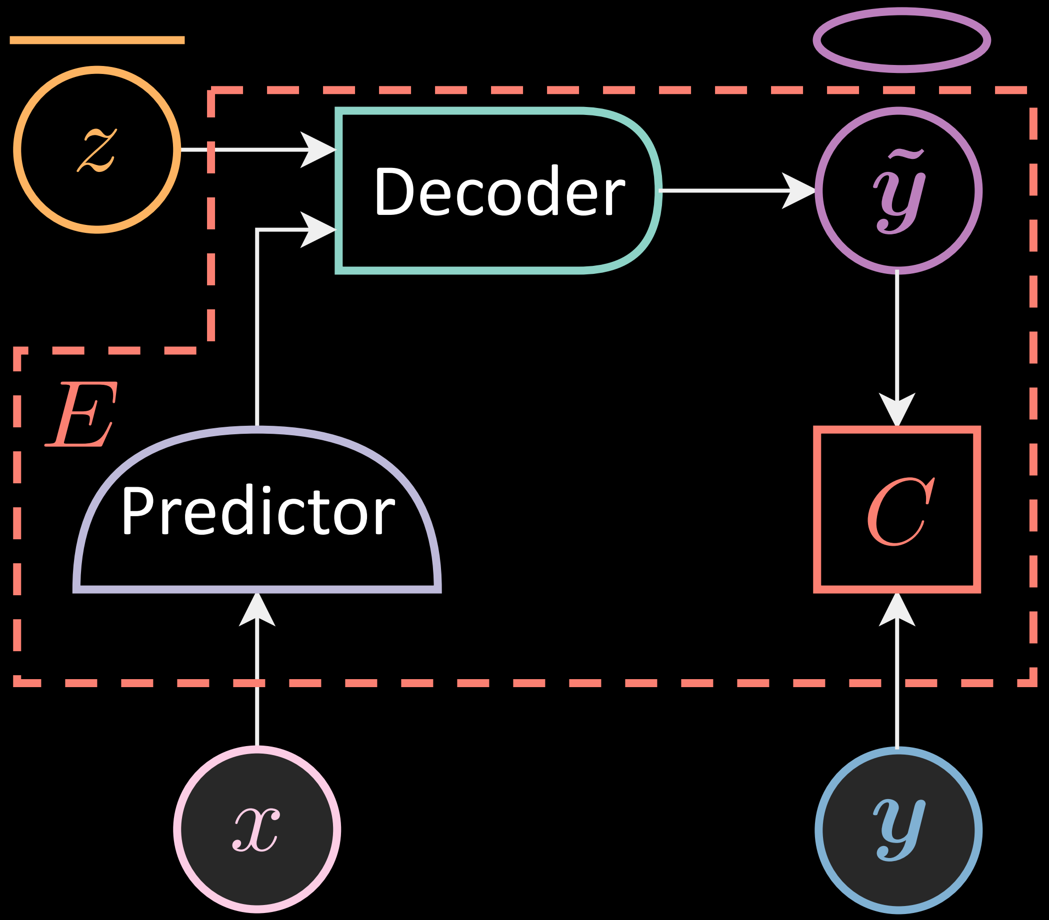




$$z = \left[0 : \frac{\pi}{24} : 2\pi\right[$$

$$x = \left[0 : \frac{1}{50} : 1\right]$$

Energy function



$$f, g : \mathbb{R} \to \mathbb{R}^2$$

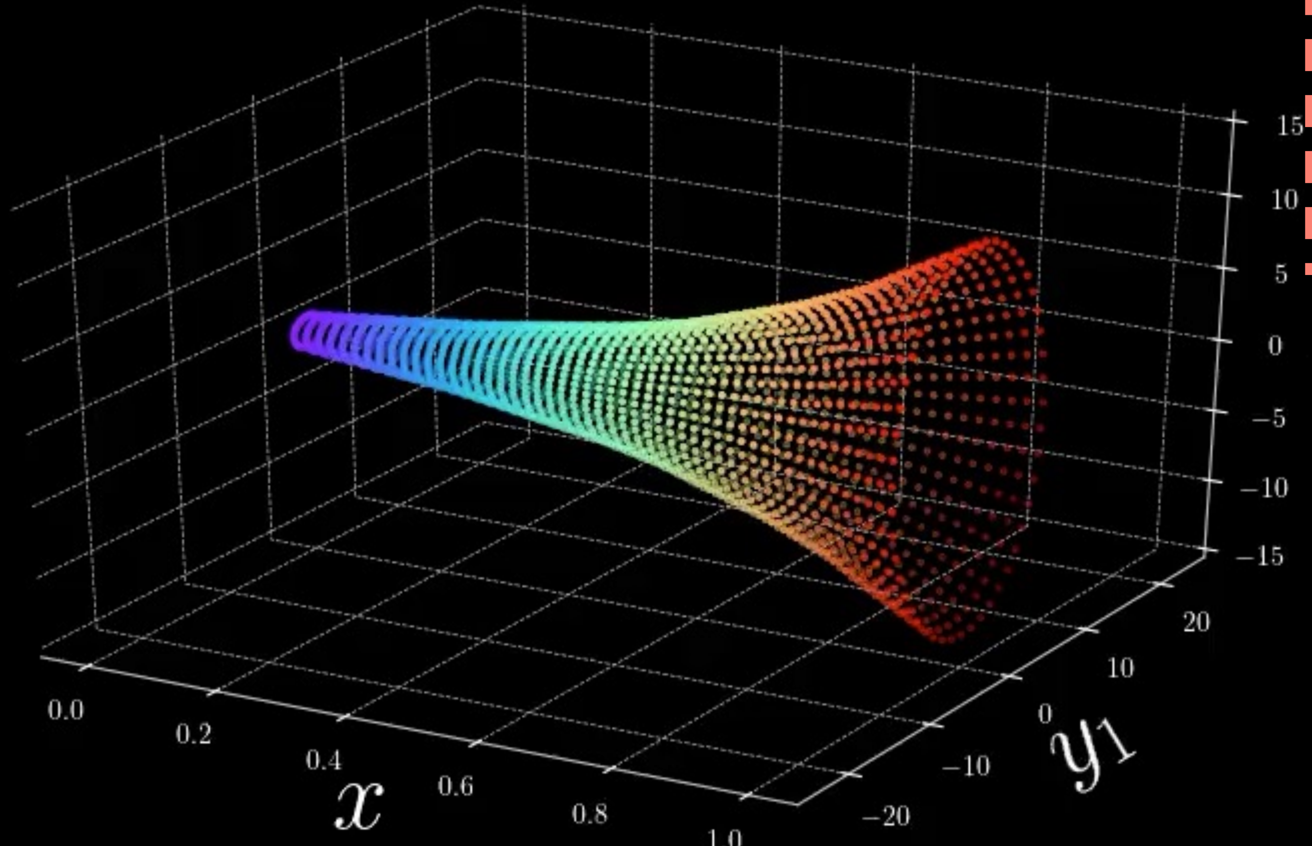
$$x \xmapsto{f} x \xrightarrow{\mathtt{L}^+} 8 \xrightarrow{\mathtt{L}^+} 8 \xrightarrow{\mathtt{L}} 2$$

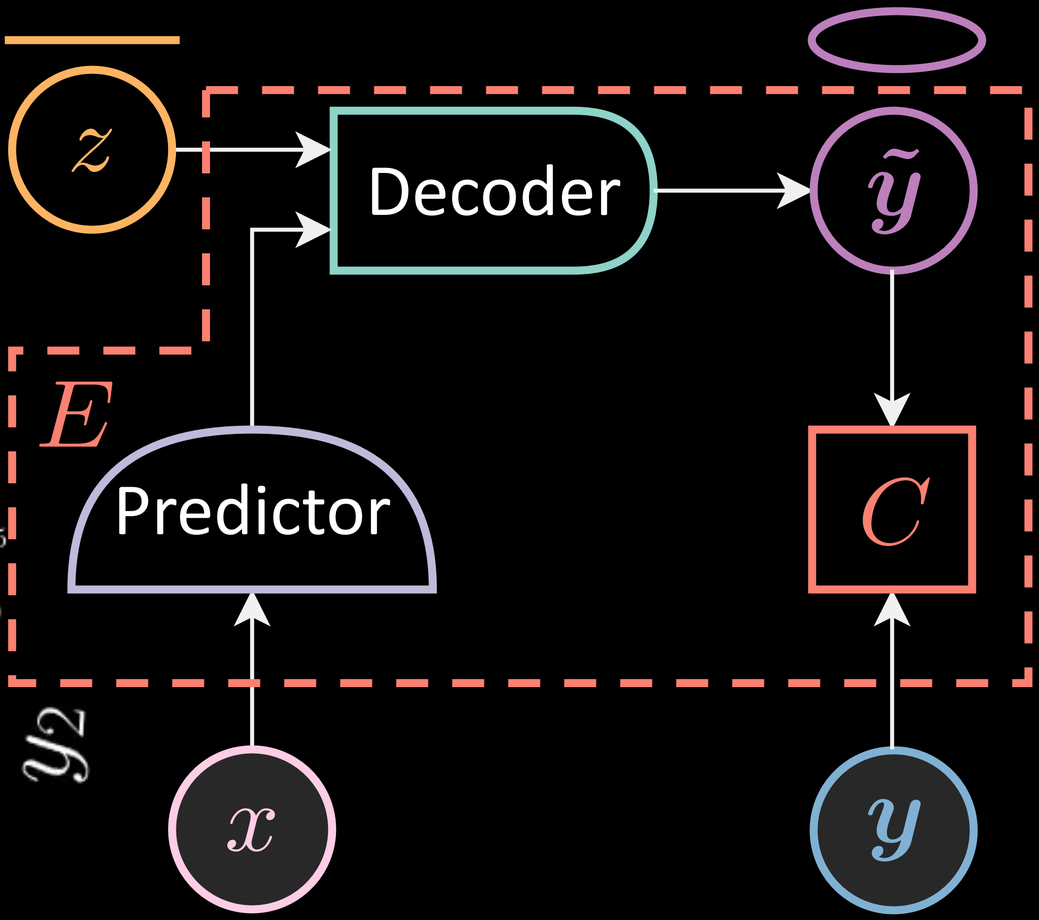
$$z \xmapsto{g} \begin{bmatrix} \cos(z) & \sin(z) \end{bmatrix}^\top$$

$$C(\boldsymbol{y}, \tilde{\boldsymbol{y}}) = \|\tilde{\boldsymbol{y}} - \boldsymbol{y}\|^2 \qquad E(x, \boldsymbol{y}, z) = C(\boldsymbol{y}, \tilde{\boldsymbol{y}})$$

$$E(x, \boldsymbol{y}, z) = [y_1 - f_1(x) g_1(z)]^2 + [y_2 - f_2(x) g_2(z)]^2$$

Trained model manifold

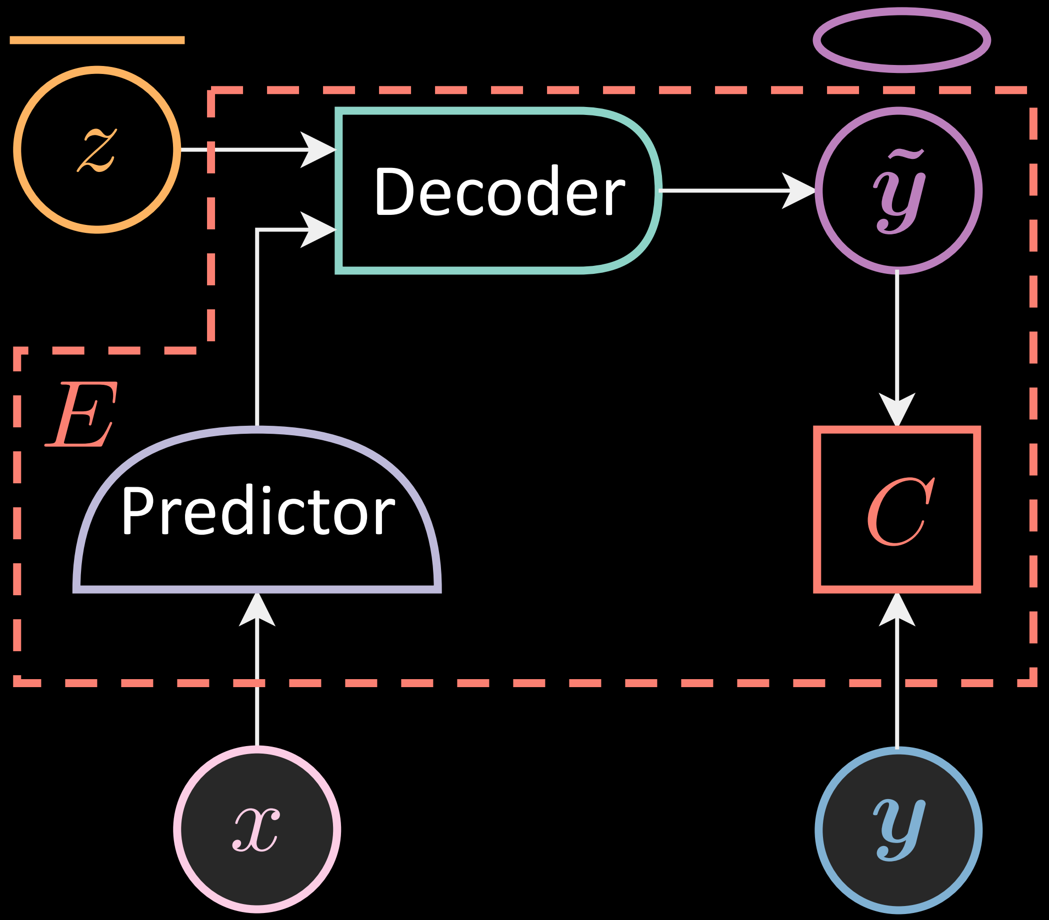




$$z = \left[0 : \frac{\pi}{24} : 2\pi\right[$$

$$x = \left[0 : \frac{1}{50} : 1\right]$$

Energy function (II)



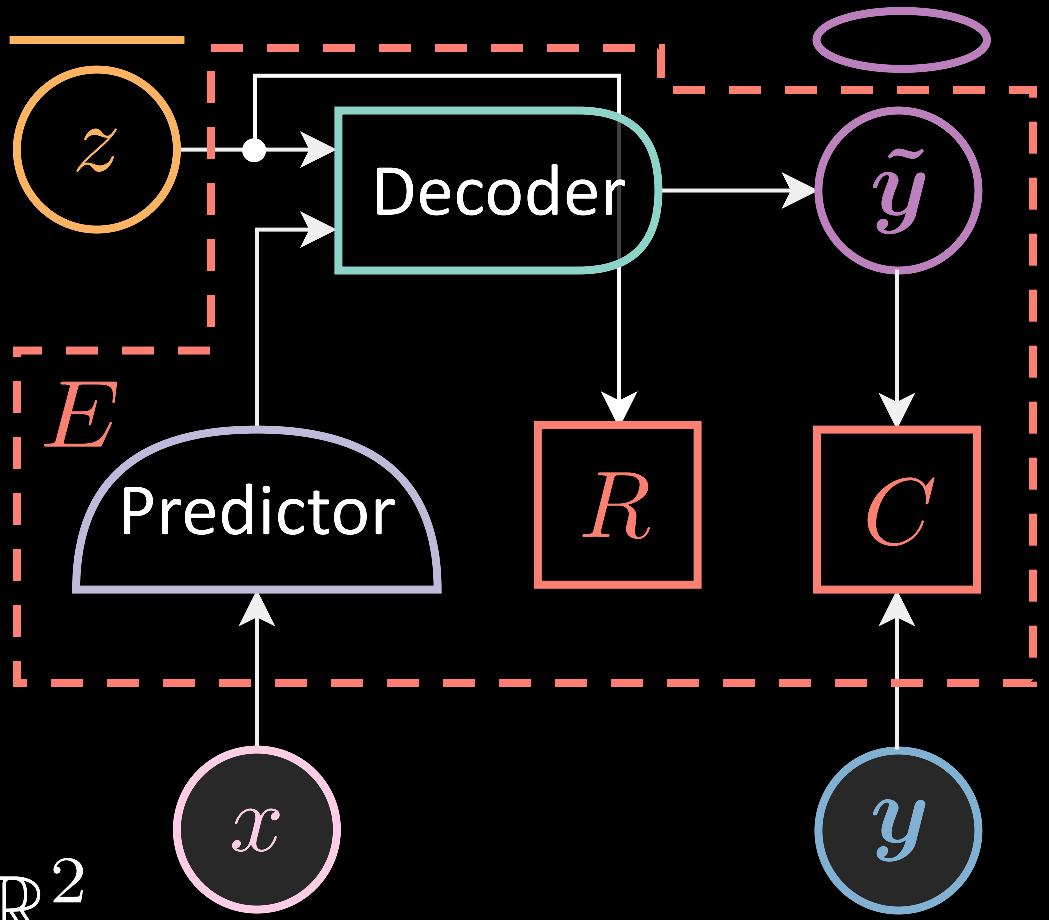
$$f : \mathbb{R} \to \mathbb{R}^{\dim(f)}$$

$$g : \mathbb{R}^{\dim(f)} \times \mathbb{R} \to \mathbb{R}^2$$

$$C(\boldsymbol{y}, \tilde{\boldsymbol{y}}) = \|\tilde{\boldsymbol{y}} - \boldsymbol{y}\|^2 \qquad E(x, \boldsymbol{y}, z) = C(\boldsymbol{y}, \tilde{\boldsymbol{y}})$$

$$E(x, \boldsymbol{y}, z) = [y_1 - g_1(f(x), z)]^2 + [y_2 - g_2(f(x), z)]^2$$

Energy function (III)



$$f : \mathbb{R} \to \mathbb{R}^{\dim(f)}$$

$$g : \mathbb{R}^{\dim(f)} \times \mathbb{R}^{\dim(z)} \to \mathbb{R}^2$$

$$C(y, \tilde{y}) = \|\tilde{y} - y\|^2 \qquad E(x, y, z) = C(y, \tilde{y}) + R(z)$$

$$E(x, y, z) = [y_1 - g_1(f(x), z)]^2 + [y_2 - g_2(f(x), z)]^2$$