Blending Physics-Based numerical simulations and seismic databases using Generative Adversarial Networks (GAN)

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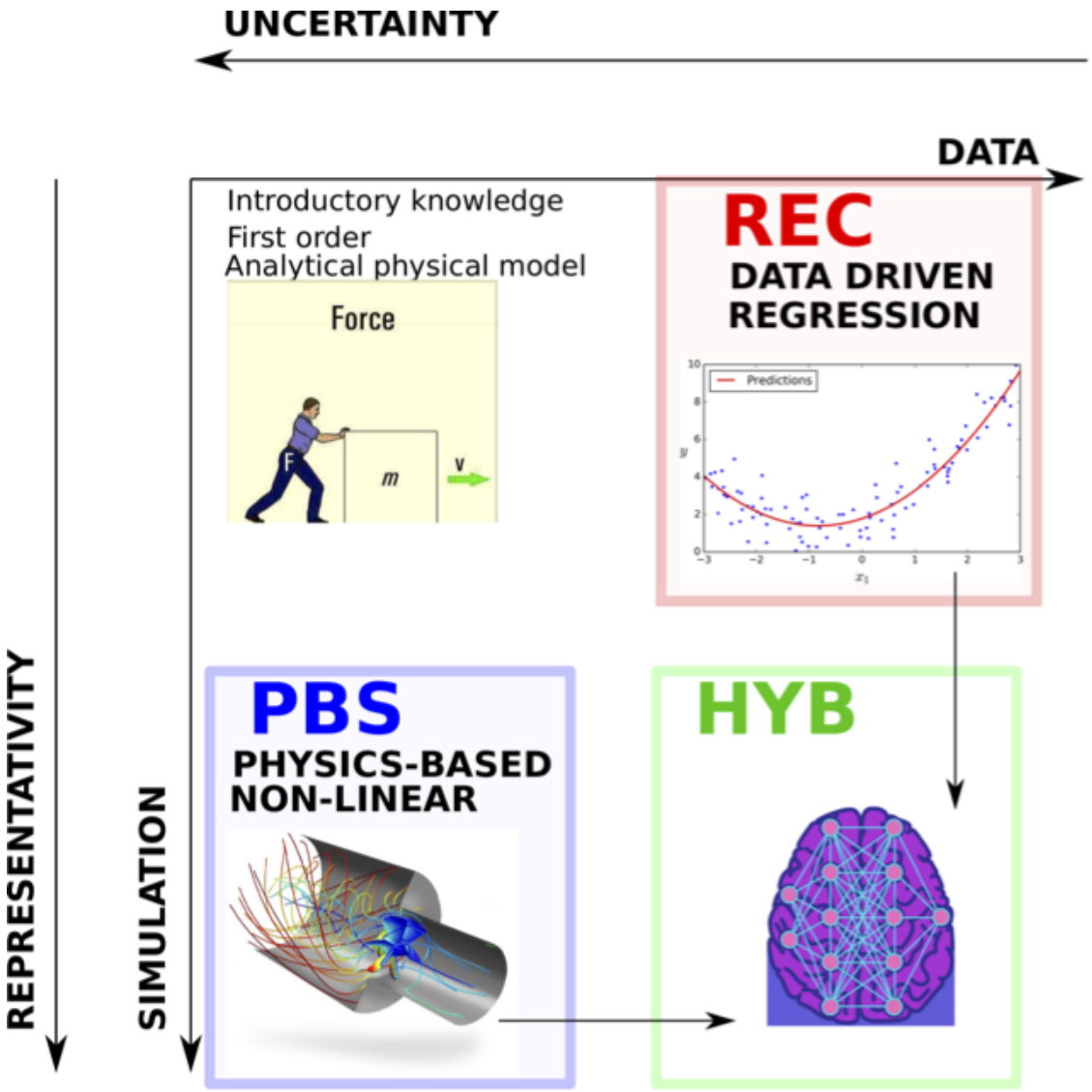
Outline

1 Make-up on Physics-based Ground motion simulation
- Hybrid models
- Seismic ground motion
- The first hybrid model

2 Deep Make-up on physics-based simulation
- Supervised learning
- Unsupervised Learning
- Generative Adversarial Networks
- Adversarial Generative auto-encoders

3 Questions
- Convergence
- Stochastic gradient

Physics-based or Data-based



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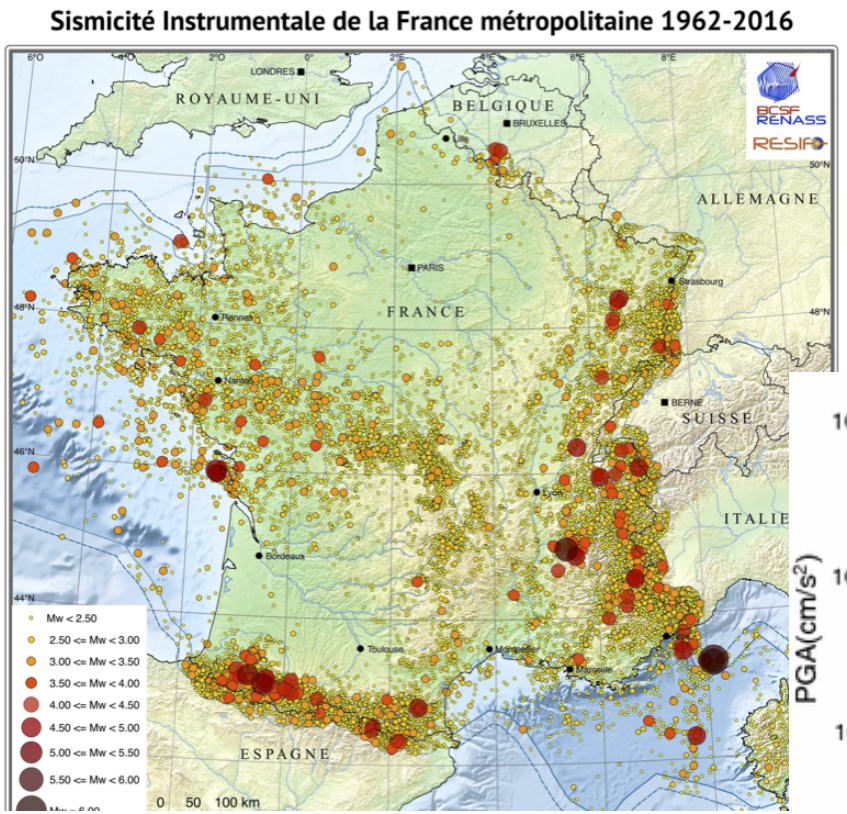
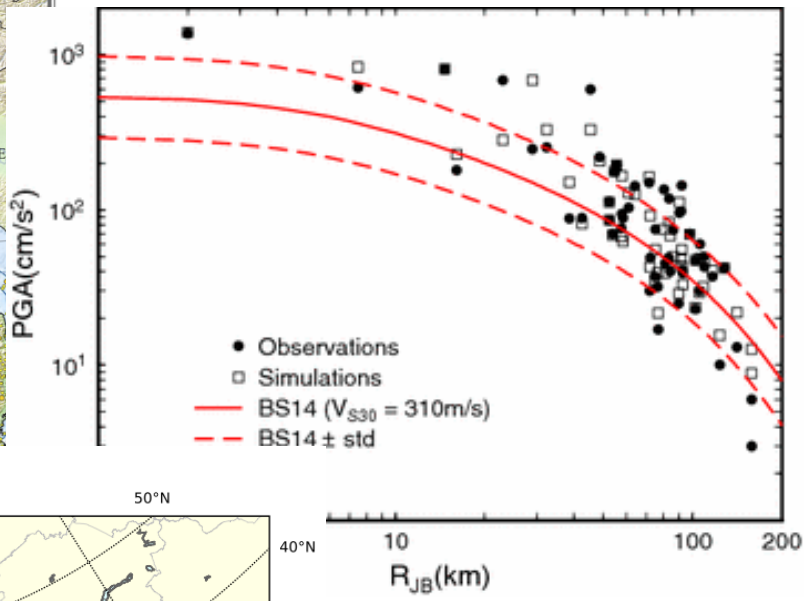
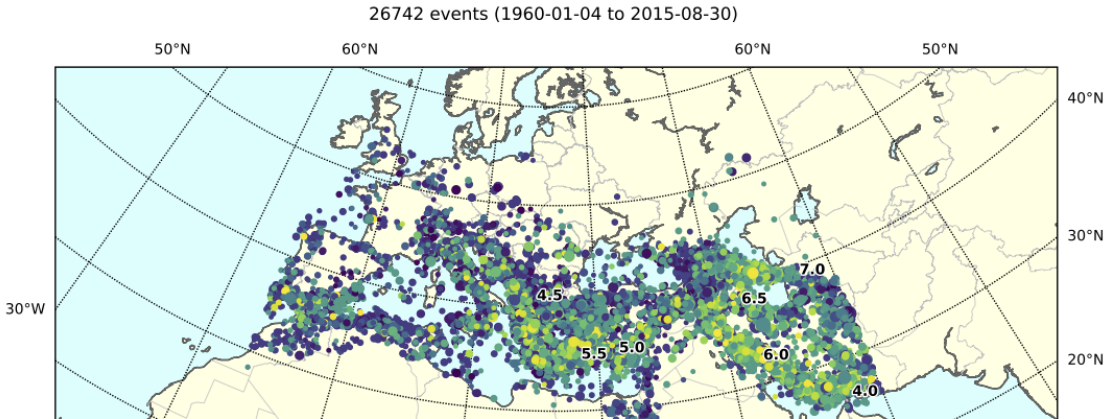
Seismic ground motion
Databases

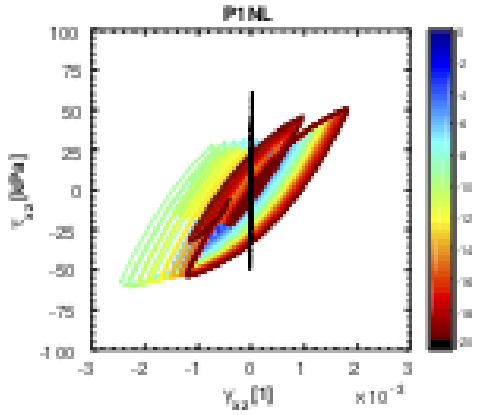


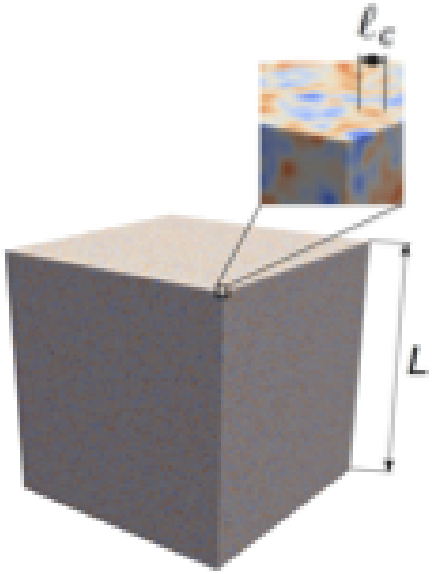


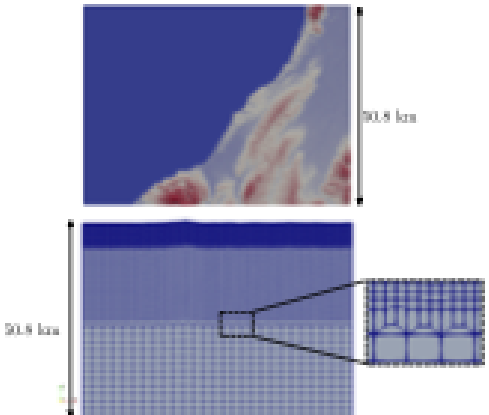


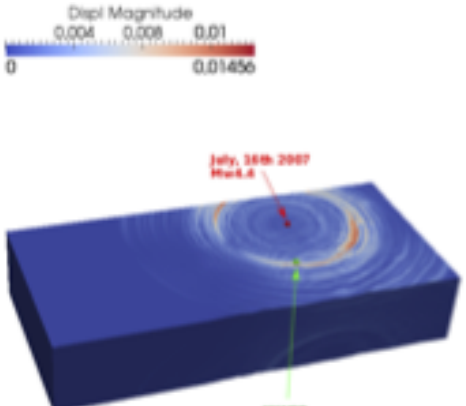
Seismic ground motion
Simulation at Low frequency

- **SEM3D**: Spectral Finite Element, Domain Decomposition, Random fields. Non-linear behavior, extended source model

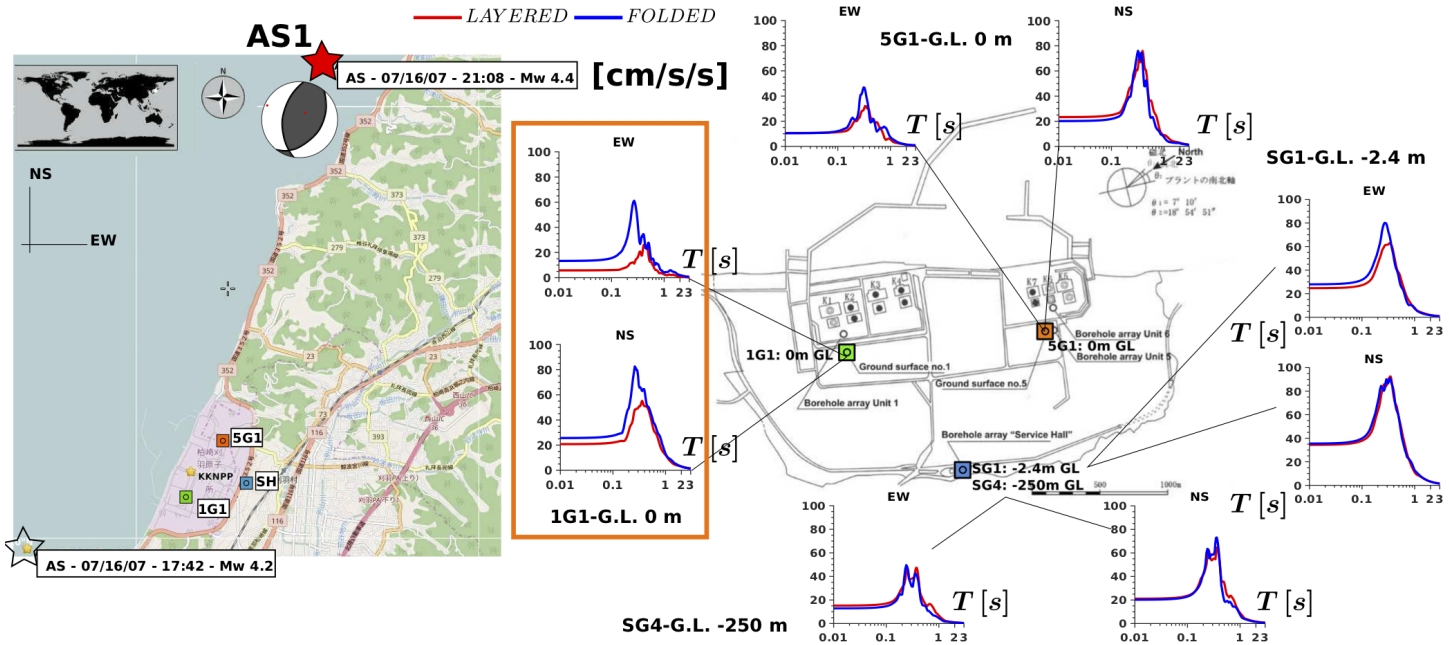








Seismic ground motion
Validation



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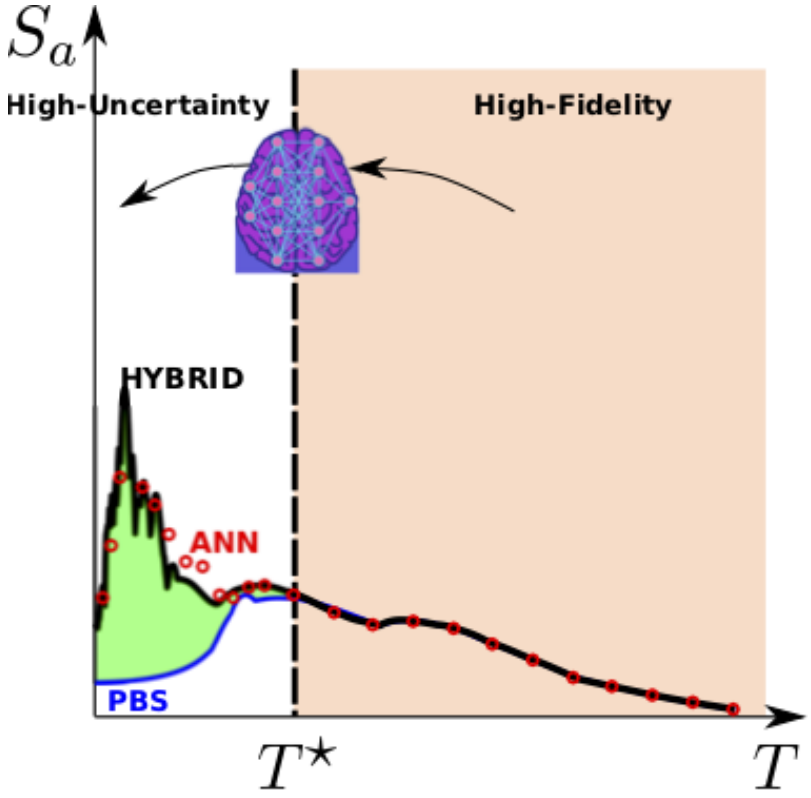
Seismic ground motion
Simulation at High Frequency

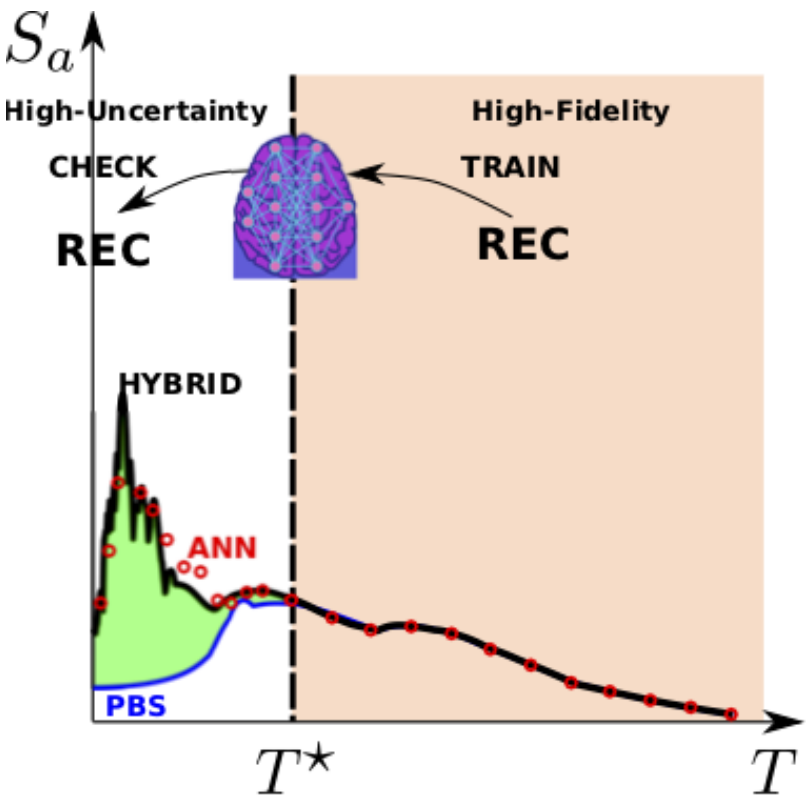
- Mapping short period spectral amplitude Y on long period ones X: $Y = H(X; W)$



$$H = h_1 \circ h_2 \qquad h_k(X) = \sigma_k(W_k X + b_k)$$

Seismic ground motion
Simulation at High Frequency

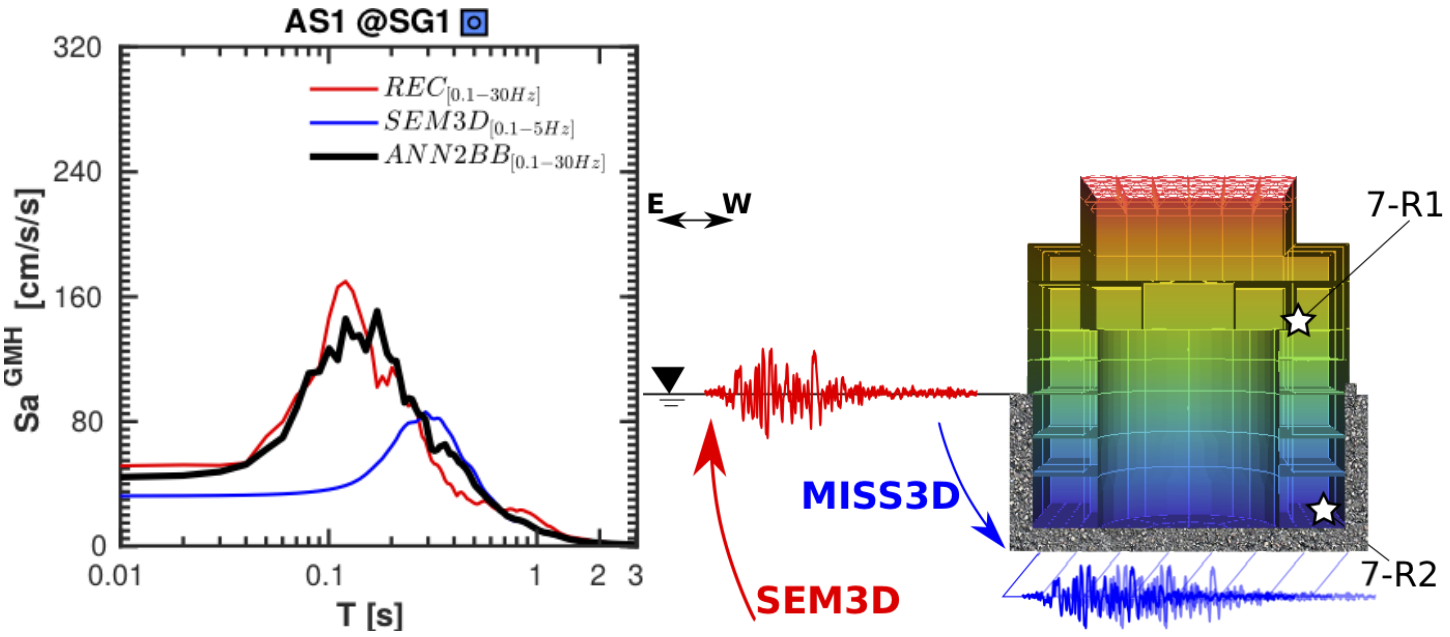
- Training on Database $(X_i, Y_i)_{i=1,m}$ Paolucci, Gatti (BSSA) 2018



$$W^* = \underset{W}{\operatorname{argmin}} \frac{1}{m} \sum_i \|Y_i - H(X_i; W)\|^2$$

Validation

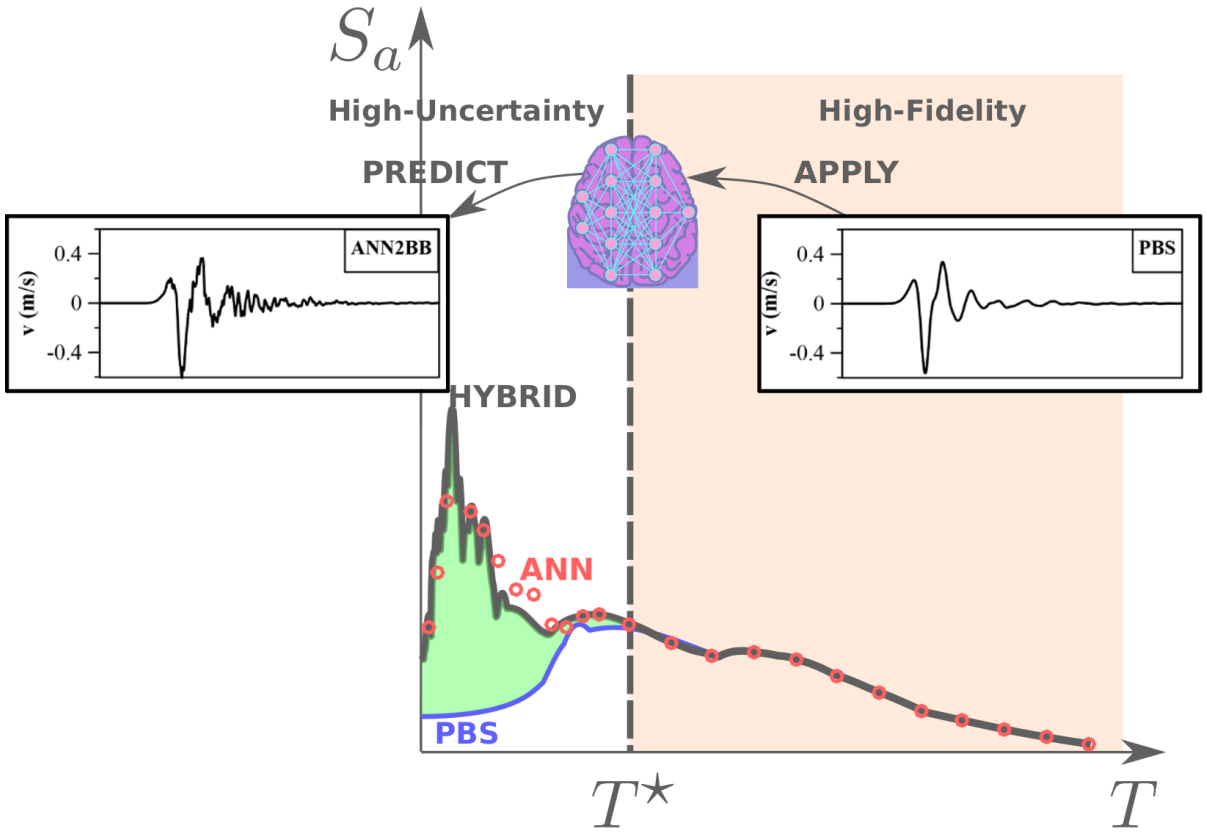
- **Kashiwazaki-Kariwa Nuclear Power Plant** (SINAPS project)

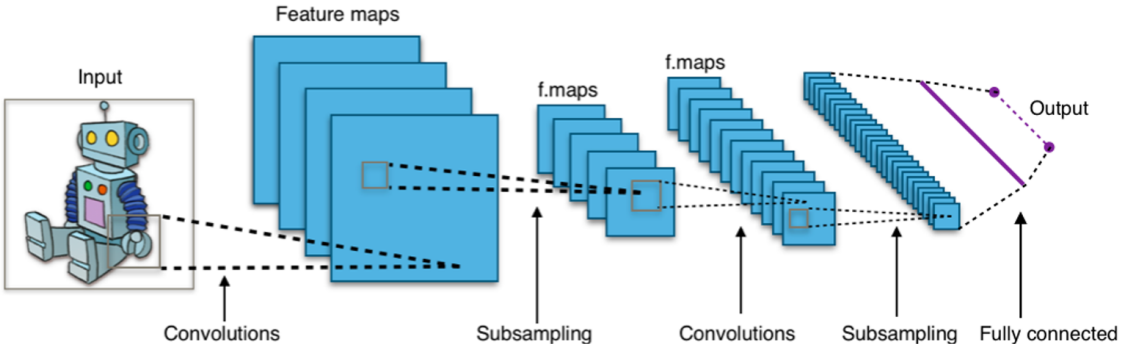


Gatti et Al. (GJI) 2018

Ground Motion simulation

Hybrid Physics-based/Databases signal processing





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Deterministic view of machine learning

- **Objective**: Identify a function based on samples:

$$\text{Find } \mathbf{h} \in \mathcal{H} \quad | \quad \mathbf{y} \approx \mathbf{h}(\mathbf{x}) \qquad \text{knowing } \mathcal{S} = \{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1,m}$$

  - **Input**: $\mathbf{x} \in \mathcal{X}$ a vector of size d (real or integer)
  - **Ouput**: $\mathbf{y} \in \mathcal{Y}$ a vector of:
    - **Labels** ($y_k \in \{"A", "B", ...\}$) : *Classification*
    - **Numbers** ($y_k \in \mathbb{R}$ or $\mathbb{Z}$): *Regression*
  - **Hypothesis**: $\mathbf{h}$ a hypothetical function in class $\mathcal{H}$

$$\mathbf{h}(\mathbf{x}) = \sigma\left(\mathbf{W}\mathbf{x} + \mathbf{b}\right)$$

  - **Sample set**: $\mathcal{S}$ of size m
  - **Deep Networks**: $\mathbf{h} = \mathbf{h}_n \circ ... \circ \mathbf{h}_1$
  - **Convolution Networks**: $W_{p+s,q+s} = W_{p,q}$
  - *Universal Approximation Theorem*

Empirical risk minimisation

- **Error/Risk/Loss function**

$$l(\mathbf{y}, \mathbf{h}(\mathbf{x})) \in \mathbb{R}^+ \qquad \text{with} \qquad l(\mathbf{y}, \mathbf{y}) = 0$$

  - **Classification** $l = \sum_k l_k$ with:
    - $l_k = 1$ when $y_k \neq h_k(\mathbf{x})$,
    - $l_k = 0$ when $y_k = h_k(\mathbf{x})$
  - **Regression**

$$l = \|\mathbf{y} - \mathbf{h}(\mathbf{x})\|_p^p$$

- **Empirical Risk**

$$L_S(\mathbf{h}) = \frac{1}{m} \sum_i l(\mathbf{y}_i, \mathbf{h}(\mathbf{x}_i))$$

- **Empirical Risk minimisation**

$$\hat{\mathbf{h}}_S = \underset{\mathbf{h} \in \mathcal{H}}{\text{argmin}}\ L_S(\mathbf{h})$$

Probabilistic approach

- Unknown probability $P(\mathrm{X},\mathrm{Y})$ on $\mathcal{D} = \mathcal{X} \times \mathcal{Y}$

$$P_{\mathrm{X}}(\mathrm{X}) = \int_{\mathcal{Y}} dP(\mathrm{X},\mathrm{Y}), \qquad P_{\mathrm{Y}|\mathrm{X}}(\mathrm{Y}|\mathrm{X}) = \frac{P(\mathrm{X},\mathrm{Y})}{P_{\mathrm{X}}(\mathrm{X})}$$

  - **Problem**: Find the *conditional probability* knowing $\mathcal{S}$

$$\hat{Q}(\mathrm{Y}|\mathrm{X}) \approx P_{\mathrm{Y}|\mathrm{X},\mathcal{S}}(\mathrm{Y}|\mathrm{X},\mathcal{S})$$

  - $\mathcal{S}$ being identically sampled: $P_{So}(\mathrm{X},\mathrm{Y}) = \frac{\mathbb{1}_{\mathcal{S}}(\mathrm{X},\mathrm{Y})}{m}$

$$Q_{So}(\mathrm{Y}|\mathrm{X}) = \frac{\mathbb{1}_{\mathcal{S}}}{m}\frac{1}{P_{So}(\mathrm{X})}, \qquad P_{So}(\mathbf{x}) = \frac{\sum_i \mathbb{1}_{\{\mathbf{x}=\mathbf{x}_i\}}}{m}$$

- **Empirical error**

$$L_{\mathcal{S}}(\hat{Q}) = \overbrace{\int_{\mathcal{D}} \ln\left(\frac{Q_{So}}{\hat{Q}}\right) P_{So} d\mathrm{X} d\mathrm{Y}}^{D_{\mathrm{KL}}(Q_{So}\|\hat{Q})} = \overbrace{\frac{-1}{m}\sum_i \ln \hat{Q}(\mathrm{Y}_i|\mathrm{X}_i)}^{\to E[-\ln \hat{Q}]}$$

Probabilistic approach
Link with the deterministic case

- **From empirical error to conditional probability**

$$Q(\mathbf{y}|\mathbf{x}) = \frac{e^{-l(\mathbf{y},\mathbf{h}(\mathbf{x}))}}{Z(\mathbf{x})}, \qquad Z(\mathbf{x}) = \int_{\mathcal{Y}} e^{-l(\mathbf{y},\mathbf{h}(\mathbf{x}))} d\mathbf{y}$$

  - Classification: $l(\mathbf{y}, \mathbf{h}(\mathbf{x})) = \mathbb{1}_{\mathbf{y} \neq \mathbf{h}(\mathbf{x})}$

$$Q(\text{"}A\text{"}|\mathbf{x}) = \frac{e^{-\mathbb{1}_{\{\text{"}A\text{"} \neq \mathbf{h}(\mathbf{x})\}}}}{Z(\mathbf{x})}, \qquad Z(\mathbf{x}) = \sum_{\mathbf{y}' \in \{\text{"}A\text{"},\ldots\}} e^{-\mathbb{1}_{\{\mathbf{y}' \neq \mathbf{h}(\mathbf{x})\}}}$$

  - L_2 Regression

$$L_D(\mathbf{h}) = E\left[L_S(Q)\right] = E\left[\frac{\|\mathbf{y} - \mathbf{h}(\mathbf{x})\|^2}{2\sigma^2}\right] + S_X(\mathbf{h})$$

Deep neural network
From data to probability

- **Converting scores to probability**
  - **Softmax** for multiple features output with individual scores $s_j(\mathbf{x})$ and total score $s = \sum_j s_j$

$$Q(y=k|\mathbf{x}) = \frac{e^{-(s-s_k)}}{\sum_j e^{-(s-s_j)}} = \frac{1}{\sum_j e^{s_j - s_k}}$$

  - **Discriminator** D for an unique feature with score $s(\mathbf{x})$ of not having the feature:

$$D(\mathbf{x}) = Q(y = \text{"0"}|\mathbf{x}) = \frac{1}{1+e^{-s}}$$

$$\begin{aligned} L_S(D) &\overset{m\to+\infty}{\to} E_{y\mathbf{x}}[-\ln Q(y|\mathbf{x})] = S(y|X) \\ &= E_{\mathbf{x}|y=\text{"0"}}[-\ln D] + E_{\mathbf{x}|y\neq\text{"0"}}[-\ln(1-D)] \\ \hat{D}(\mathbf{x}) &= \underset{D}{\operatorname{argmin}}\ L_S(D) \end{aligned}$$

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Auto-encoders
And convolution networks

- **Autoencoder**

$$\mathbf{z} = F(\mathbf{x}), \qquad \mathbf{y} = G(\mathbf{z}), \qquad S = \{\mathbf{x}_i, \mathbf{y}_i = \mathbf{x}_i\}_{i=1,m}$$

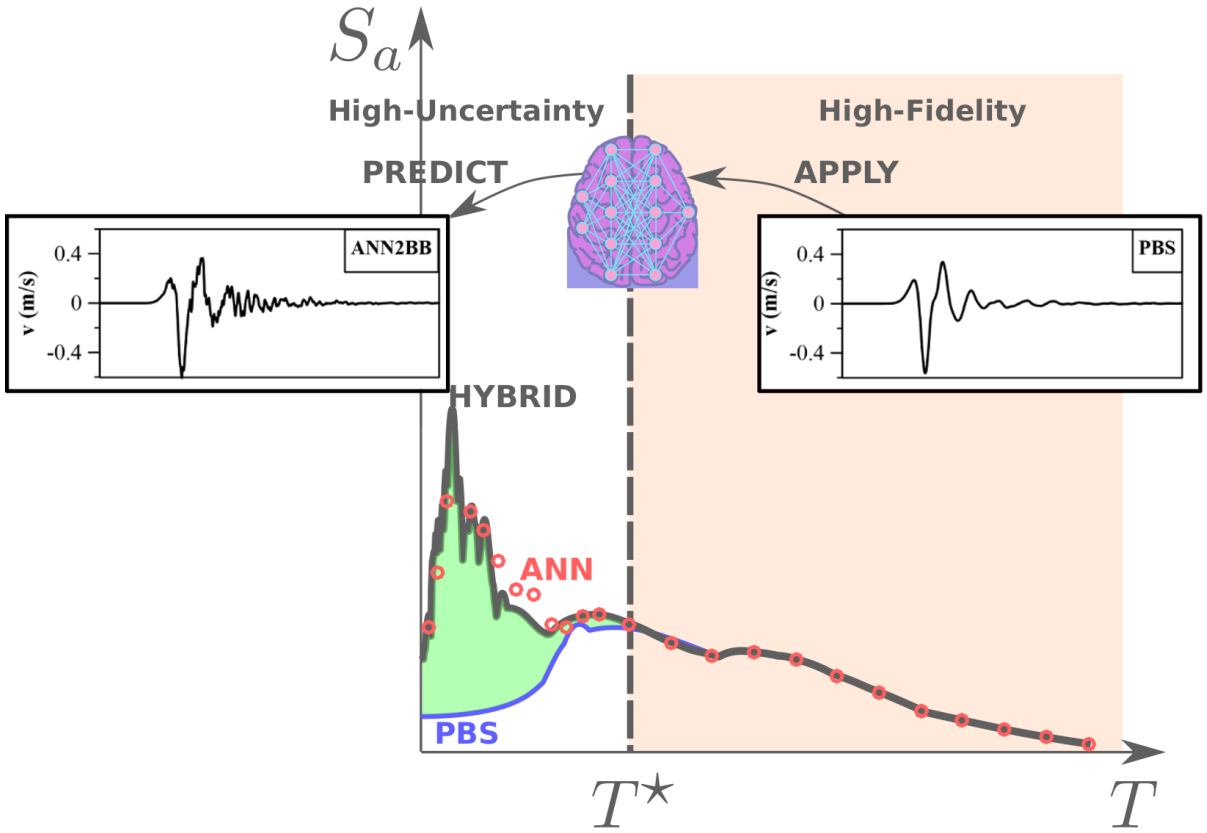
$$L_S(F,G) = \sum_i \|\mathbf{x}_i - F(G(\mathbf{x}_i))\|^2$$

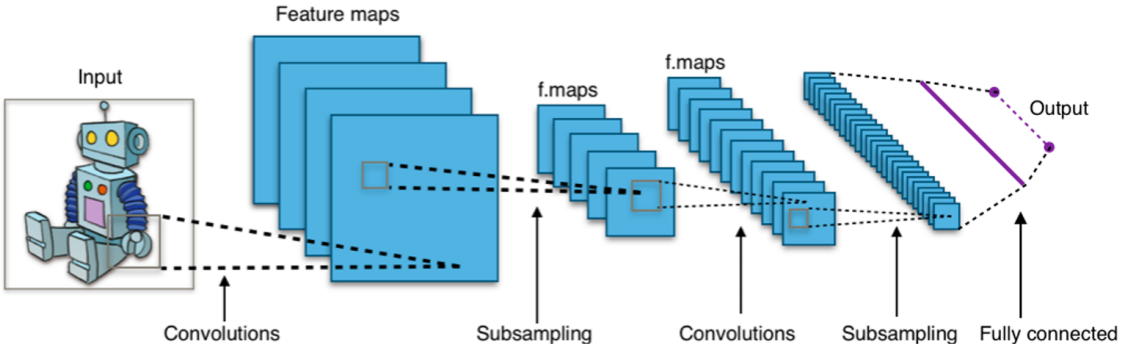
$$(\hat{F}, \hat{G}) = \underset{F,G}{\text{argmin}}\ L_S(F,G)$$

  - $\mathcal{Z} = F(\mathcal{X})$ is smaller than $\mathcal{X}$
  - Noise is added to the input
  - Weights are linked when $F = G^{-1}$: $\mathbf{W}_F = \mathbf{W}_G^T$
  - F and G can have several layers and be convolutional
- *Remark:* In the linear case
  - **Convolutional case**: F is any Wavelet transform
  - **full case**: G is any Karhunen-Loeve or POD
  - *Weakness*: P_{Z} is not simple

Ground Motion simulation

Hybrid Physics-based/Databases signal processing





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Generative Adversarial Networks (GAN)
Conditional Entropy

- **Mixture Probability of**
  - $\mathbf{x}_1 \in \mathcal{X}$ with distribution p_1
  - $\mathbf{x}_2 \in \mathcal{X}$ with distribution p_2.
  - $\mathbf{y} \in \{"1", "2"\}$ with respective probability α and $1-\alpha$
  - $(\mathbf{x}, \mathbf{y})$ with $p(.|\mathbf{y} = "1") = p_1$ and $p(.|\mathbf{y} = "2") = p_2$

$$p(\mathbf{x}) = \alpha p_1(\mathbf{x}) + (1-\alpha) p_2(\mathbf{x})$$

  - $\hat{D}(\mathbf{x}) = p(\mathbf{y} = "1"|\mathbf{x})$
- Entropy

$$S(\mathbf{x}, \mathbf{y}) = \underbrace{S(\mathbf{x}|\mathbf{y})}_{\alpha S(\mathbf{x}_1) + (1-\alpha) S(\mathbf{x}_2)} + S(\mathbf{y}) = S(\mathbf{y}|\mathbf{x}) + S(\mathbf{x})$$

- Cross-Information

$$\begin{aligned} I(\mathbf{x}, \mathbf{y}) &= S(\mathbf{y}) - S(\mathbf{y}|\mathbf{x}) \geq 0 \\ S(\mathbf{y}|\mathbf{x}) &= \alpha E_{x_1}\left(-\ln \hat{D}\right) + (1-\alpha) E_{x_2}\left(-\ln(1-\hat{D})\right) \end{aligned}$$

Generative Adversarial Networks (GAN)

Jensen-Shannon Divergence

- **Mixture Probability of**
  - $\mathbf{x}_1 \in \mathcal{X}$ with distribution p_1
  - $\mathbf{x}_2 \in \mathcal{X}$ with distribution p_2.
  - $\mathbf{y} \in \{1, 2\}$ with respective probability α and $1 - \alpha$
  - $(\mathbf{x}, \mathbf{y})$ with $p(\mathbf{x}|\mathbf{y} = 1) = p_1(\mathbf{x})$ and $p(\mathbf{x}|\mathbf{y} = 2) = p_2(\mathbf{x})$

$$p(\mathbf{x}) = \alpha p_1(\mathbf{x}) + (1 - \alpha) p_2(\mathbf{x})$$

  - $D(\mathbf{x}) = p(\mathbf{y} = 1|\mathbf{x})$
- **Jensen-Shannon Divergence** as cross information:

$$\begin{aligned} S(\mathbf{y}) - S(\mathbf{y}|\mathbf{x}) &= S(\mathbf{x}) - S(\mathbf{x}|\mathbf{y}) = \\ D_{\mathrm{JS}}(\mathbf{x}_1 \| \mathbf{x}_2) &= \alpha E_{\mathbf{x}_1}\left[\ln \frac{p_1}{p}\right] + (1 - \alpha) E_{\mathbf{x}_2}\left[\ln \frac{p_2}{p}\right] \\ &= \alpha D_{\mathrm{KL}}(p_1 \| p) + (1 - \alpha) D_{\mathrm{KL}}(p_2 \| p) \end{aligned}$$

Generative Adversarial Networks (GAN)

Empirical error I

- **Finding the best model $\mathbf{x}_m$ for data $\mathbf{x}_d$**

$$\hat{\mathbf{x}}_m = \underset{\mathbf{x}_m}{\operatorname{argmin}}\ D_{\mathrm{JS}}(\mathbf{x}_d \| \mathbf{x}_m)$$

  - Finding $D_{\mathrm{JS}}(\mathbf{x}_d \| \mathbf{x}_m)$ estimate based on empirical data
  - Finding a minimum (Stochastic gradient).

- $(-D_{\mathrm{JS}})$ as the entropy of conditional probability [1] $p(\mathbf{y} \in \{"d", "m"\} | \mathbf{x})$:

$$S(\mathbf{y}|\mathbf{x}) \quad = \quad -D_{\mathrm{JS}}(\mathbf{x}_d \| \mathbf{x}_m) + S(Y)$$

[1]

$$p(\mathbf{y}|\mathbf{x}) = \frac{p(\mathbf{x}|\mathbf{y})p(\mathbf{y})}{p(\mathbf{x})} = \alpha \frac{p(\mathbf{x}_d)}{p(\mathbf{x})} \text{ or } (1-\alpha)\frac{p(\mathbf{x}_m)}{p(\mathbf{x})}$$

Generative Adversarial Networks (GAN)

Empirical error II

- D_{JS} as the conditional probability $p(\mathbf{y}\in\{"d","m"\}|\mathbf{x})$

$$S(\mathbf{y}|\mathbf{x}) \quad = \quad -D_{\mathrm{JS}}(\mathbf{x}_d\|\mathbf{x}_m) + S_\alpha$$

- Find a discriminator $\hat{D}(\mathbf{x})$ such that $\hat{D}(\mathbf{x}) = P("d"|\mathbf{x})$:

$$S(\mathbf{y}|\mathbf{x}) = -\alpha E\left[\ln \hat{D}\right] - (1-\alpha)E\left[\ln(1-\hat{D})\right]$$

- Estimation of D as a **discriminator** with a classification Neural Network (max Log Likelihood):

$$\hat{D} = \underset{D}{\mathrm{argmax}}\ \frac{1}{m}\sum_i \ln D(\mathbf{x}_i)$$

Generative Adversarial Networks (GAN)
Implementation

- **A random unit-centered-Gaussian vector z**
- **The generator**: $\mathbf{x}_m = G(\mathbf{z})$
- **The Discriminator**: $D(\mathbf{x}) \in [0,1]$
- **The mixture sampler**: $S = \{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1,m}$ with $\mathbf{x}_i \in \{\mathbf{x}_d, G(\mathbf{z})\}$ with probability α and $1-\alpha$

$$\hat{G} = \underset{G}{\operatorname{argmin}} \max_{D} \quad \alpha E_d \left[\ln D(\mathbf{x}_d)\right] + (1-\alpha) E_z \left[\ln(1 - D(G(\mathbf{z}))]\right)$$

- **Properties**
  - $\hat{G}$ minimise the distance (JS-Divergence) between the modeled and the data distributions
  - $\hat{G}$ maximise the conditional entropy $S(Y|X)$

Goodfellow 2014

Generative Adversarial Networks (GAN)

Strength and weakness

$$\hat{G} = \underset{G}{\operatorname{argmin}} \max_{D} \quad \alpha E_d \left[\ln D(\mathbf{x}_d)\right] + (1-\alpha) E_m \left[\ln(1 - D(G(\mathbf{z}_m)))\right])$$

- **Strength**
  - Identification of a representation model of sampled data using independent unit random seeds $\mathbf{z}$
  - A Polynomial Chaos Expansion (PCE) can be built when $\mathbf{z}$ is a unit Gaussian random vector

$$\mathbf{x}_m = \sum_j \mathbf{x}_j \psi_j(\mathbf{z}) \quad , \quad \mathbf{x}_j = \int G(\mathbf{z}) \psi_j(\mathbf{z}) \nu(\mathbf{z}) d\mathbf{z}$$

- **Weaknesses** (same as PCE)
  - Non uniqueness
  - $\mathbf{z}$ is a collection of hidden features
  - No encoding algorithm ($\mathbf{z} = F(\mathbf{x})$)

Adversarial Encoder (GAN)

- Mixture between $\mathbf{z}_d = F(\mathbf{x}_d)$ and unitary $\mathbf{z}_m$ with $D_z = P(Y = "m"|\mathbf{z})$

$$\begin{aligned} -S(Y|Z) &= (1-\alpha)E_m(\ln D_z) + \alpha E_d(\ln(1 - D_z(F(.))) \\ &= D_{JS}(p_{z_m}||p_{z_d}) - S(Y) \end{aligned}$$

$$\begin{aligned} \hat{F} = \underset{F}{\operatorname{argmin}} \max_{D_z} \quad & \alpha E_d\left[\ln(1 - D_z(F(\mathbf{x}_d)))\right] \\ + \quad & (1-\alpha)E_z\left[\ln D_z\right] \end{aligned}$$

- **Weakness**
  - Marginals on $\mathbf{x}$ and $\mathbf{z}$ are equally distributed but their joint probabilities are not. Hence:

$$\mathbf{x}_d \neq G(F(\mathbf{x}_d)) \quad , \quad \mathbf{z} \neq F(G(\mathbf{z}))$$

  - No link between encoder and generator when learning.

Bidirectional GAN

- **biGAN**: $\hat{D}_{xz}(\mathbf{x},\mathbf{z}) \approx P(\text{"}m\text{"}|(\mathbf{x},\mathbf{z}))$

$$
\begin{aligned}
(\hat{F},\hat{G},\hat{D}_{xz}) &= \underset{F,G}{\operatorname{argmax}}\ \underset{D_{xz}}{\operatorname{argmin}}\ L_S(D_{xz},F,G) \\
L_S(D_{xz},F,G) &= \frac{-1}{m}\sum_i (\ln D_{xz}(G(\mathbf{z}_i),\mathbf{z}_i))\mathbb{1}_{y_i=\text{"}m\text{"}} \\
&\quad + \ln(1-D_{xz}(\mathbf{x}_i,F(\mathbf{x}_i)))\mathbb{1}_{y_i=\text{"}d\text{"}}) \\
&\approx S(Y|X,Z)
\end{aligned}
$$

- **Weakness**
  - Sample set does not cover all $\mathcal{X}\times\mathcal{Z}$ space

$$\mathbf{x}_d \neq G(F(\mathbf{x}_d)) \qquad , \qquad \mathbf{z} \neq F(G(\mathbf{z}))$$

  - Need to better control $S(X|Z)\to 0$ or $\mathbf{x}_d - G(F(\mathbf{x}_d)$.

Donahue, Dumoulin 2017

Cycling GAN
ALICE

- $\hat{D}_{xz}(\mathbf{x}, \mathbf{z}) \approx P(\text{"}m\text{"}|(\mathbf{x}, \mathbf{z}))$

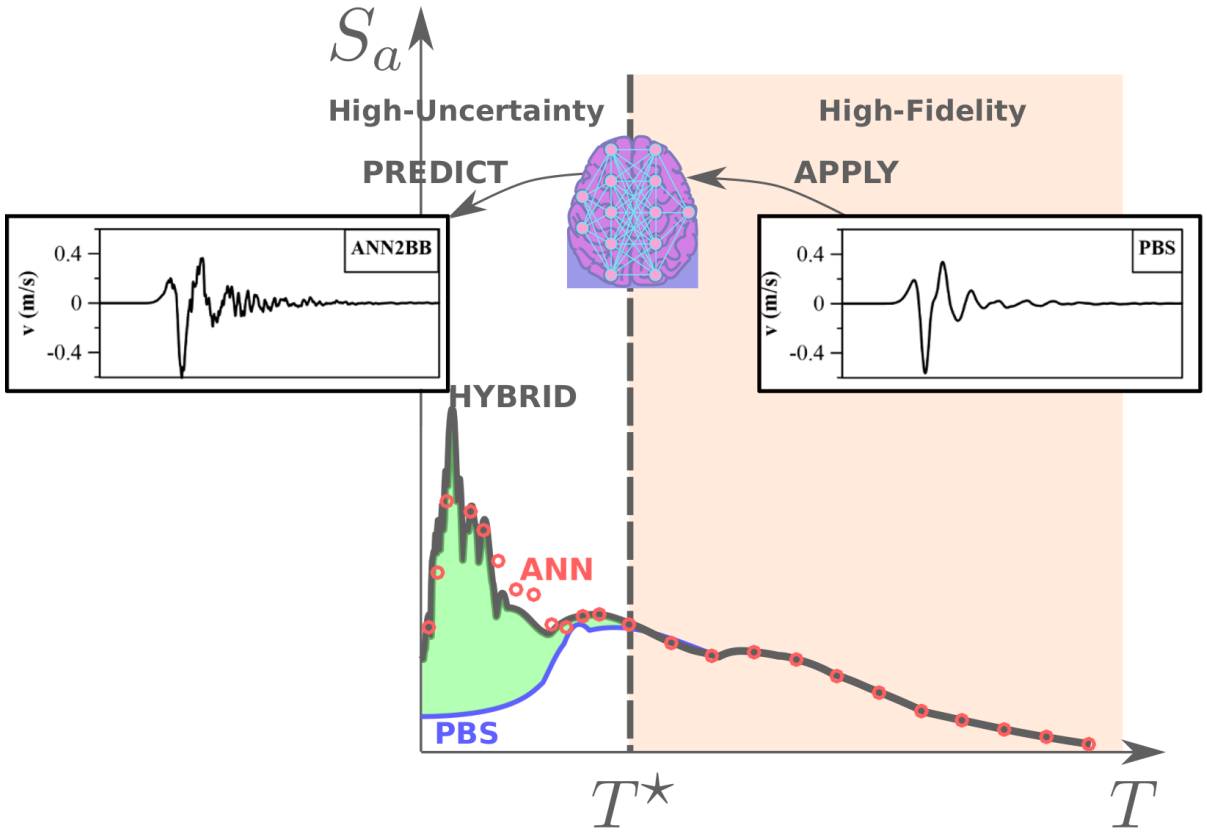
$$
\begin{aligned}
(\hat{F}, \hat{G}, \hat{D}_{xz}) &= \underset{F,G}{\operatorname{argmax}} \ \underset{D_{xz}}{\operatorname{argmin}} \ L_S^*(D_{xz}, F, G) \\
L_S^*(D_{xz}, F, G) &= L_S(D_{xz}, F, G) + \eta \|\mathbf{x}_d - G(F(\mathbf{x}_d))\|_p^p
\end{aligned}
$$

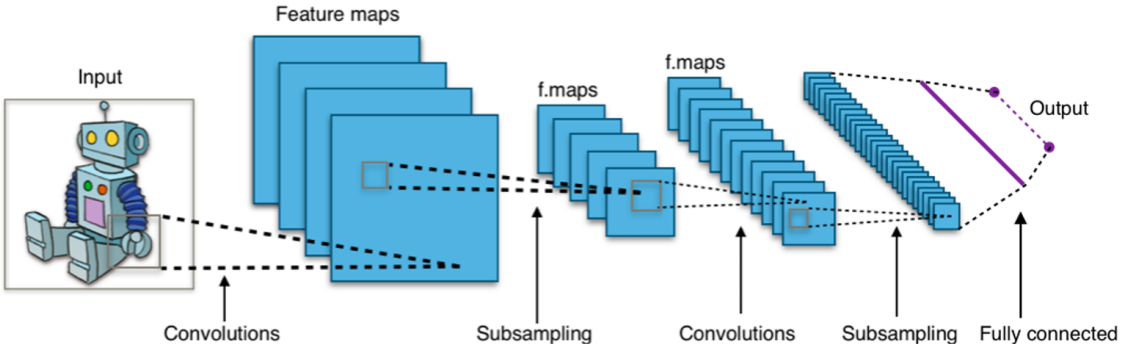
- **Strength**
  - It works (!)
  - Filtering $\|\mathbf{x}_d - G(F(\mathbf{x}_d)\|_p^p$ gives broadband output for filtered inputs.
  - Use of GAN to discriminate $\mathbf{x}_d \neq G(F(\mathbf{x}_d))$.

Li et Al. 2017

Ground Motion simulation

Hybrid Physics-based/Databases signal processing





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Adversarial Generative auto-encoders

- **Encoder**: $\mathbf{z}_1 = F(\mathbf{x})$
- **Generator**: $\mathbf{z} = (\mathbf{z}_1, \mathbf{z}_2)$ with $\mathbf{z}_2$ Gaussian

$$\mathbf{x}_m = G(\mathbf{z})$$

- **Optimisation**

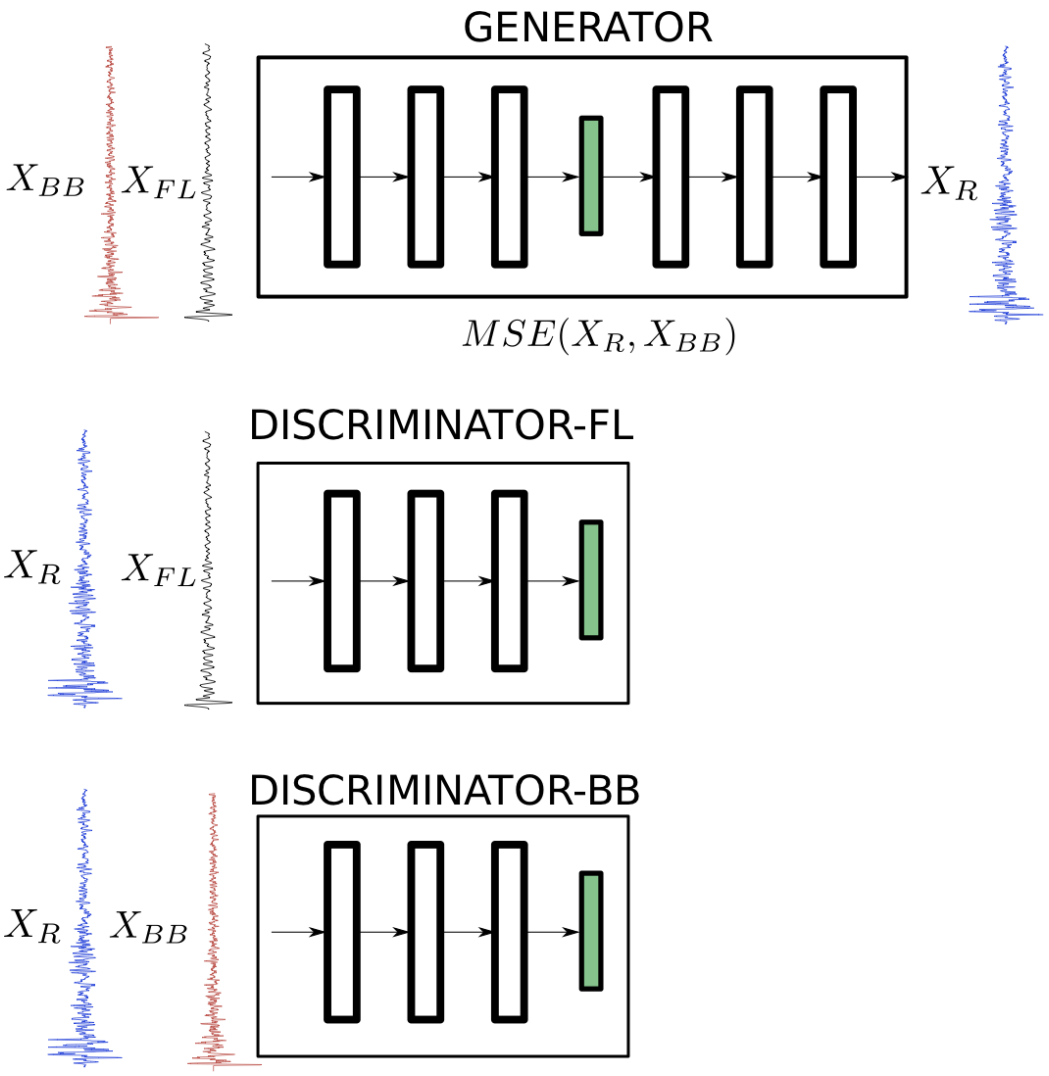
$$(\hat{F}, \hat{G}) = \underset{(G,F)}{\operatorname{argmin}} \underbrace{L_S(G,F)}_{\frac{1}{m}\sum_i \|\mathbf{x}_i - G(\mathbf{z}_i)\|^2}$$

  - D discriminator between data $\mathbf{x}_d$ and model $\mathbf{x}_m$:

$$\begin{aligned}(\hat{F}, \hat{G}) &= \underset{(G,F)}{\operatorname{argmin}} \left(L_S(G,F)\right. \\ &\quad + \max_D \left(E_d\left[\ln D(\mathbf{x}_d)\right] + E_m\left[\ln D(G(\mathbf{z}))\right]\right)\end{aligned}$$

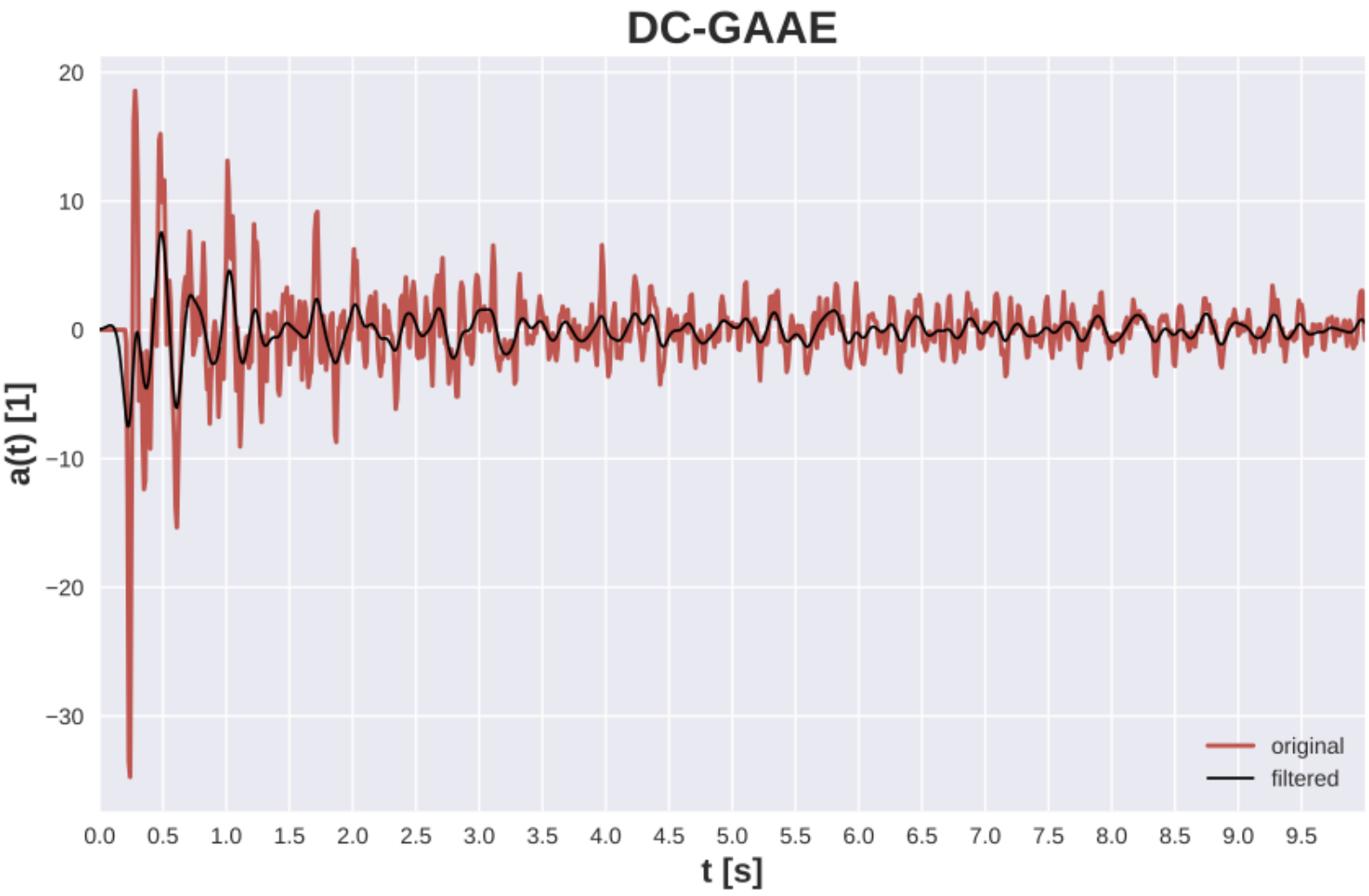
Ground Motion simulation

Hybrid Physics-based/Databases Adversarial Generative auto-encoders



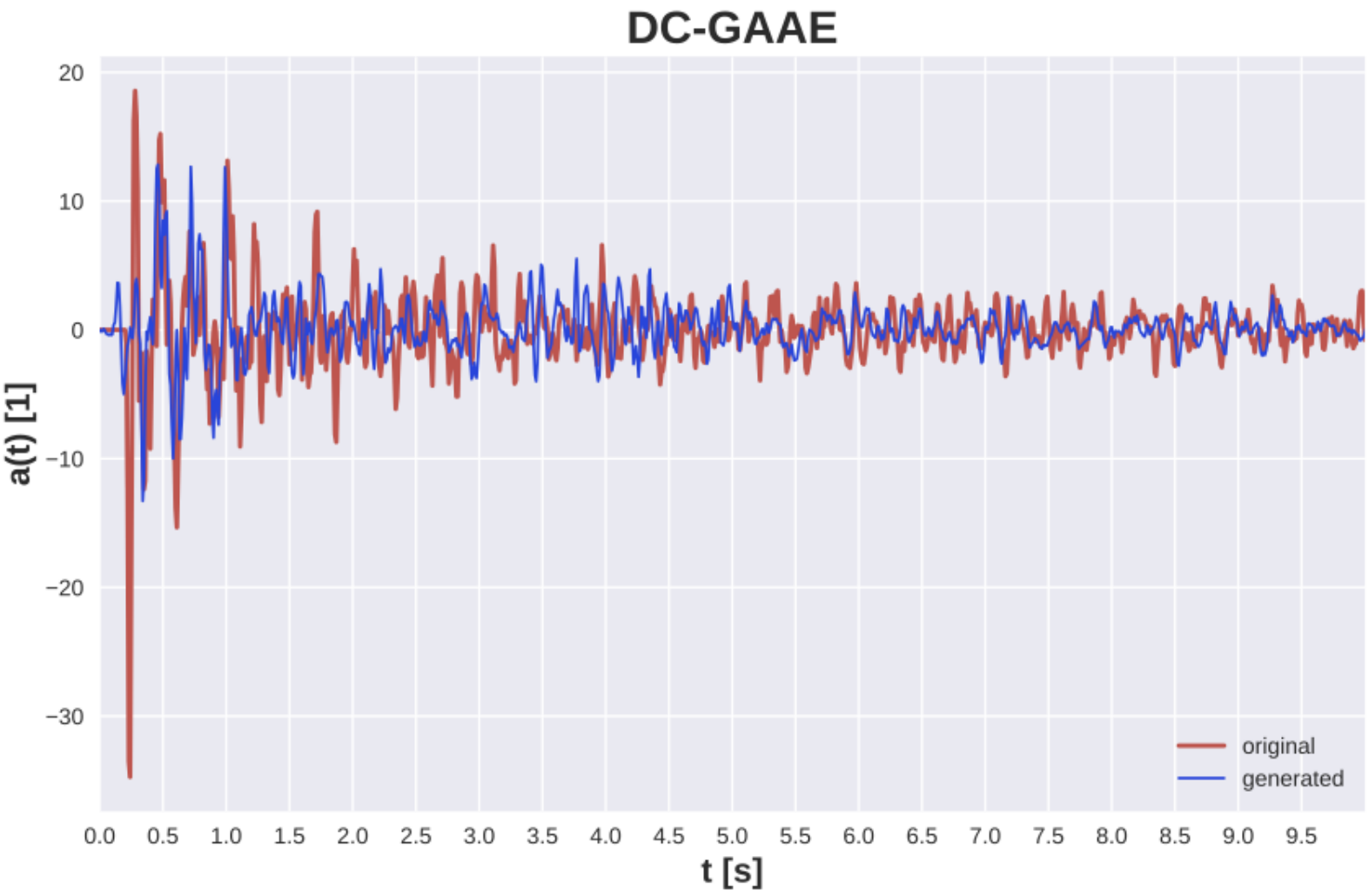
Ground Motion simulation

Hybrid Physics-based/Databases Adversarial Generative auto-encoders



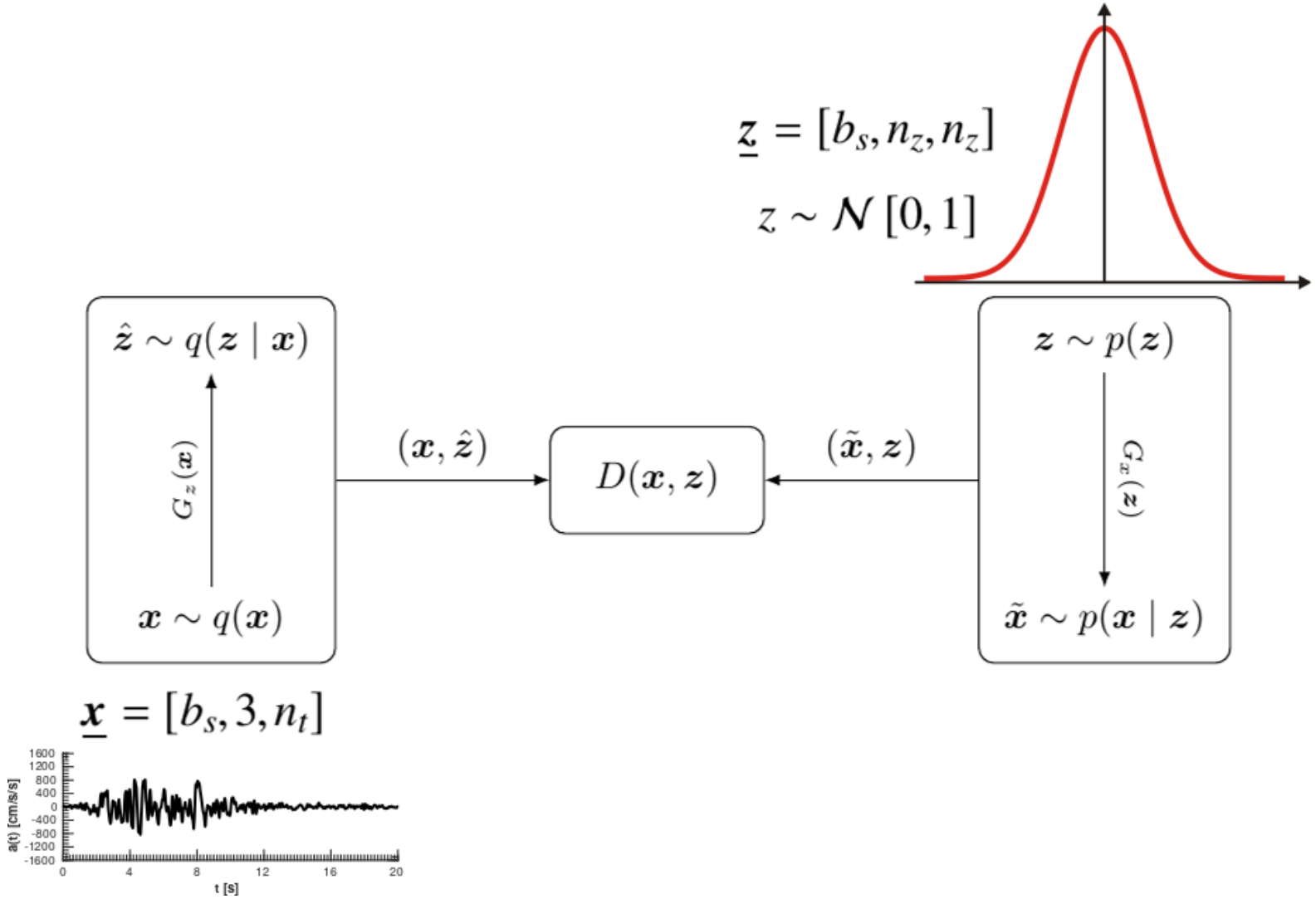
Ground Motion simulation

Hybrid Physics-based/Databases Adversarial Generative auto-encoders



Ground Motion simulation

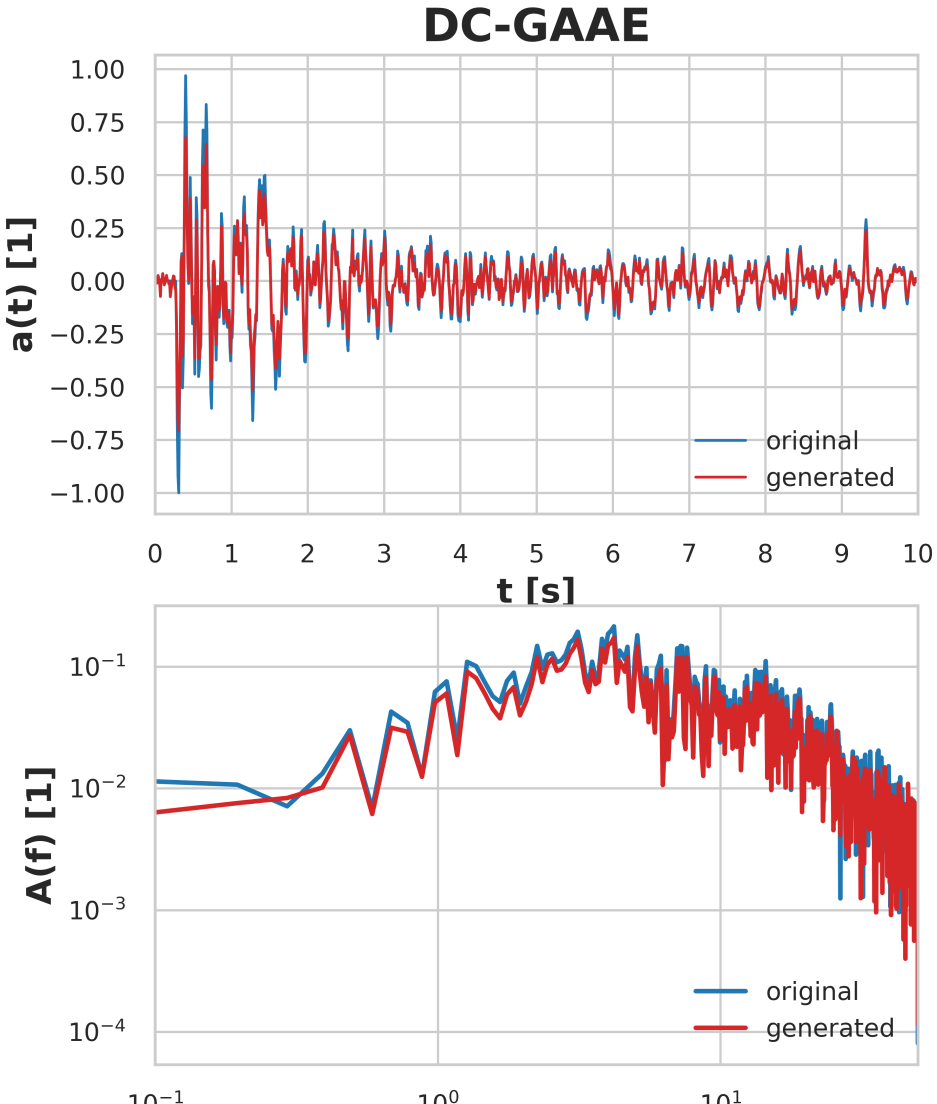
Hybrid Physics-based/Databases signal processing: ALICE like



Ground Motion simulation

Hybrid Physics-based/Databases signal processing: ALICE like

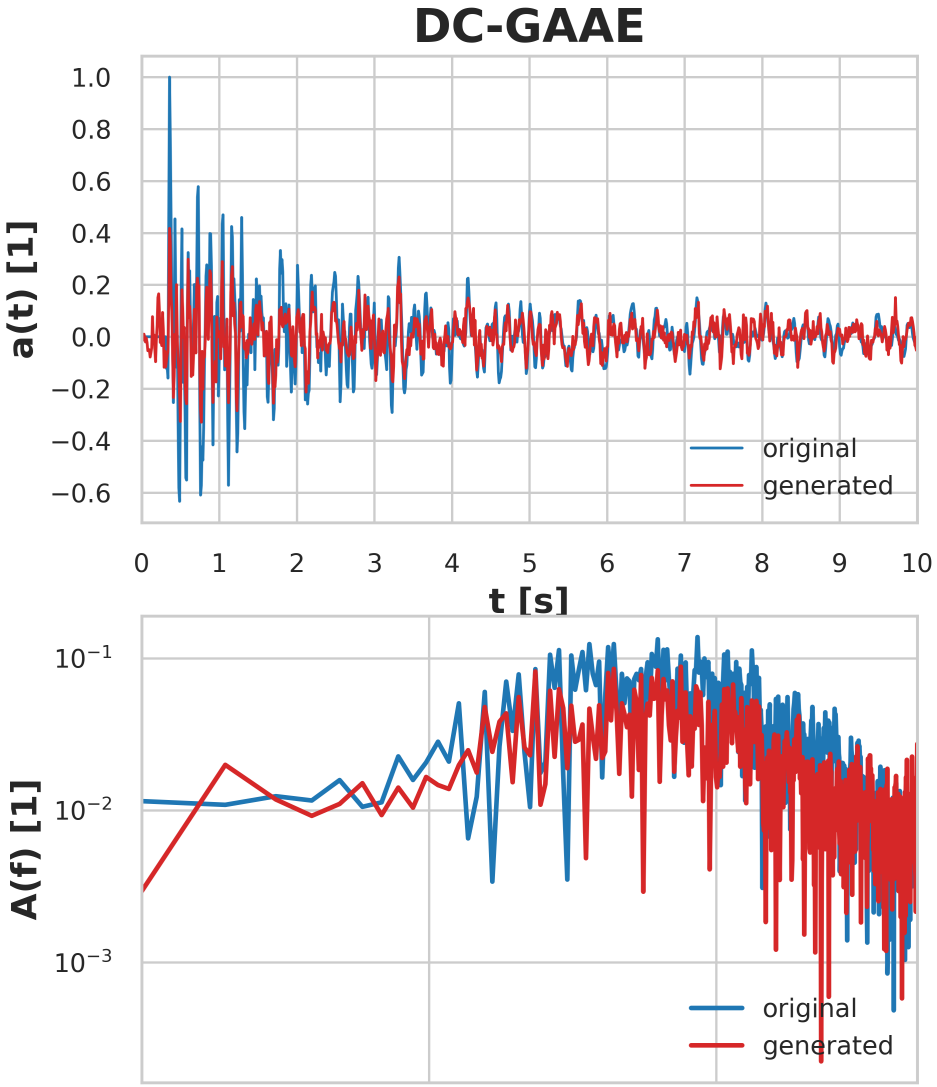
Signal reconstruction



Ground Motion simulation

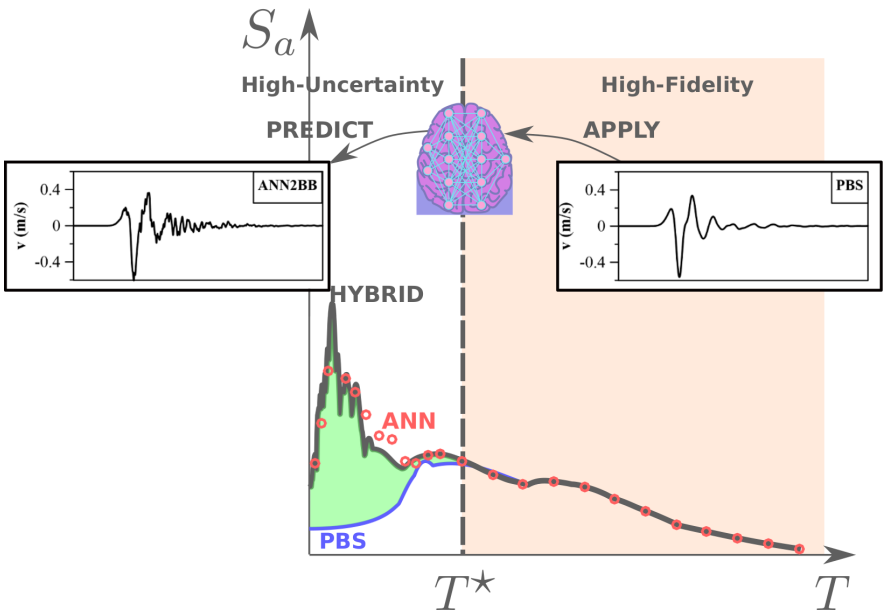
Hybrid Physics-based/Databases signal processing: ALICE+

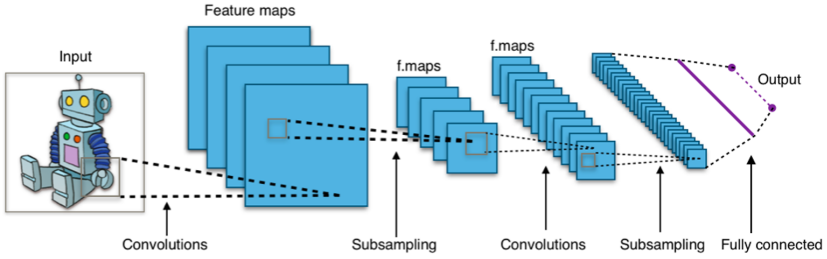
Signal generation from filtered input



Ground Motion simulation

Hybrid Physics-based/Databases signal processing





Thank you !

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Empirical risk minimisation
Discussion

- **Empirical Risk minimisation**

$$\hat{\mathbf{h}}_S = \underset{\mathbf{h}\in\mathcal{H}}{\operatorname{argmin}}\ L_S(\mathbf{h}), \qquad L_S(\mathbf{h}) = \frac{1}{m}\sum_i l(\mathbf{y}_i, \mathbf{h}(\mathbf{x}_i))$$

- **Difficulties**
  - **Ill-posed**: no-uniqueness, smoothness and convexity are required for optimisation methods
  - **Under and Overfitting**:
    - $L_D(\mathbf{h})$ the "true error" (to be defined)
    - $\mathbf{h}_D$ the "best hypothesis" on $\mathcal{H}$ (to be defined)

$$\mathbf{h}_D = \underset{\mathbf{h}\in\mathcal{H}}{\operatorname{argmin}}\ L_D(\mathbf{h})$$

$$L_D(\mathbf{h}_D) \leq L_D(\hat{\mathbf{h}}_S), \qquad L_S(\hat{\mathbf{h}}_S) \leq L_S(\mathbf{h}_D)$$

  - Approximation and generalisation errors

$$L_D(\hat{\mathbf{h}}_S) = \underbrace{L_D(\mathbf{h}_D)}_{\underset{|\mathcal{H}|\to+\infty}{\to} 0} + \underbrace{\Big(L_D(\hat{\mathbf{h}}_S) - L_D(\mathbf{h}_D)\Big)}_{\leq c\sqrt{\frac{|\mathcal{H}|}{m}}}$$

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Stochastic gradient

- **Assumption**: $L_S(\mathbf{h}) = L_S(\mathbf{W})$ is smooth and locally convex ($l = \frac{1}{2}\|\mathbf{y} - \mathbf{h}(\mathbf{x})\|^2$)

$$\nabla_{\mathbf{W}} L_S = \frac{1}{m} \sum_i \nabla_{\mathbf{W}} \mathbf{h}(\mathbf{x}_i) \cdot \underbrace{\nabla_{\mathbf{h}} l(\mathbf{y}_i, \mathbf{h}(\mathbf{x}_i))}_{\Delta_i = \mathbf{y}_i - \mathbf{h}(\mathbf{x}_i)}$$

$$\nabla_{\mathbf{W}} \mathbf{h}(\mathbf{x}) \Delta = \prod_{l=1}^{n} \nabla_{\mathbf{W}_l} \mathbf{h}_l(\mathbf{x}_l) \cdot \Delta_l$$

$$\nabla_{\mathbf{W}_l} \mathbf{h}_l(\mathbf{x}_l) = g_l' \left(\mathbf{W}_l \mathbf{x}_l + \mathbf{b}_l\right) \mathbf{x}_l \Delta_l$$

- **Stochastic gradient**

$$\mathbf{W}^{(j+1)} = \mathbf{W}^{(j)} + \underbrace{\alpha}_{\text{Learning rate}} \nabla_{\mathbf{W}} \mathbf{h}(\mathbf{x}_i) \Delta_i$$

Probabilistic approach
Log-Likelihood

- **Log-Likelihood** of S

$$L_{\hat{Q}}(S) = -L_S(\hat{Q}) \quad = \quad \frac{1}{m}\sum_i \ln \hat{Q}(\mathrm{Y}_i|\mathrm{X}_i) - \mathrm{cst}$$

- **Log-Likelihood Maximisation**

$$\hat{Q}_S = \underset{Q\in\mathcal{Q}}{\operatorname{argmax}}\ L_Q(S)$$

- **Generalisation error**

$$\begin{aligned} L_D(Q) &= E\left[D_{\mathrm{KL}}(P\|QP_{\mathrm{X}})\right] \\ &= E\left[-\ln Q(\mathrm{Y}|\mathrm{X})\right] - \overbrace{S(P_{\mathrm{Y}|\mathrm{X}})}^{\text{Entropy of } P_{\mathrm{Y}|\mathrm{X}}} \end{aligned}$$

  - **Consistency**

$$L_D(Q) = E\left[L_S(Q)\right]$$