Interpretable Machine Learning

Learning to Explain

Learning goals

- Optimization problems in hard-masking
- **•** Generative masking
- Sampling-based instance-wise feature selection

INSTANCE-WISE FEATURE SELECTION

- What happens when we do not have explanation data?
- Need to use the task-specific supervision signal to create explanations
- Key principle: Given an instance, automatically learn to select features during inference from the task-specific supervised signal

INSTANCE-WISE FEATURE SELECTION

- Key principle: Given an instance, automatically learn to select features during inference
- The selected features can be implemented as a binary mask over the original feature space
- Selector network selects the mask, predictor network predicts using the masked input

PROBLEMS IN OPTIMISATION

- Selector network selects the mask, predictor network predicts using the masked input
- Binary masking introduces discontinuity in the neural network
- \bullet Discontinuity \rightarrow gradient-based optimisation is not possible
- How can we learn the parameters of such a network using gradient-based optimization?

GENERATIVE MASKS

- Masks are generated from a probability distribution
- Instance-wise feature selection as finding the expectation of the predictor function distributed according to human interpretability

$$
\mathcal{F}(\boldsymbol{\theta}) := \int p(\mathbf{m}; \mathbf{x}, \boldsymbol{\theta}) f(\mathbf{m} \odot \mathbf{x}; \boldsymbol{\phi}) \mathrm{d} \mathbf{x} = \mathbb{E}_{p(\mathbf{m}; \mathbf{x}, \boldsymbol{\theta})} [f(\mathbf{m} \odot \mathbf{x}; \boldsymbol{\phi})]
$$

INSTANCE-WISE FEATURE SELECTION

- The distribution over explanations is parameterized by a neural network
- The predictor network is also parameterized by a neural network

$$
\mathcal{F}(\boldsymbol{\theta}) := \int p(\mathbf{m}; \boldsymbol{\theta}) f(\mathbf{m} \odot \mathbf{x}; \boldsymbol{\phi}) \mathrm{d} \mathbf{x} = \mathbb{E}_{p(\mathbf{m}; \boldsymbol{\theta})} [f(\mathbf{m} \odot \mathbf{x}; \boldsymbol{\phi})]
$$

• Predictor network accepts a masked input

MONTE CARLO SAMPLING

$$
\mathcal{F}(\boldsymbol{\theta}) := \int p(\mathbf{m}; \mathbf{x}, \boldsymbol{\theta}) f(\mathbf{m} \odot \mathbf{x}; \boldsymbol{\phi}) \mathrm{d} \mathbf{x} = \mathbb{E}_{p(\mathbf{m}; \mathbf{x}, \boldsymbol{\theta})} [f(\mathbf{m} \odot \mathbf{x}; \boldsymbol{\phi})]
$$

Trick: $\nabla_{\boldsymbol{\theta}} \log p(\mathbf{x}; \boldsymbol{\theta}) = \frac{\nabla_{\boldsymbol{\theta}} p(\mathbf{x}; \boldsymbol{\theta})}{p(\mathbf{x}; \boldsymbol{\theta})}$

 \rightsquigarrow In a simplified notation (ignoring **m**), we get the following:

$$
\eta := \nabla_{\theta} \mathcal{F}(\theta) = \nabla_{\theta} \mathbb{E}_{p(\mathbf{x};\theta)}[f(\mathbf{x}; \phi)]
$$

\n
$$
= \nabla_{\theta} \int p(\mathbf{x}; \theta) f(\mathbf{x}) d\mathbf{x} = \int f(\mathbf{x}) \nabla_{\theta} p(\mathbf{x}; \theta) d\mathbf{x}
$$

\n
$$
= \int p(\mathbf{x}; \theta) f(\mathbf{x}) \nabla_{\theta} \log p(\mathbf{x}; \theta) d\mathbf{x}
$$

\n
$$
= \mathbb{E}_{p(\mathbf{x}; \theta)} [f(\mathbf{x}) \nabla_{\theta} \log p(\mathbf{x}; \theta)]
$$

MONTE CARLO ESTIMATOR

$$
\mathcal{F}(\boldsymbol{\theta}) := \int p(\mathbf{m}; \mathbf{x}, \boldsymbol{\theta}) f(\mathbf{m} \odot \mathbf{x}; \boldsymbol{\phi}) d\mathbf{x} = \mathbb{E}_{p(\mathbf{m}; \mathbf{x}, \boldsymbol{\theta})} [f(\mathbf{m} \odot \mathbf{x}; \boldsymbol{\phi})]
$$

$$
\boldsymbol{\eta} := \nabla_{\boldsymbol{\theta}} \mathcal{F}(\boldsymbol{\theta}) = \nabla_{\boldsymbol{\theta}} \mathbb{E}_{p(\mathbf{x};\boldsymbol{\theta})}[f(\mathbf{x};\boldsymbol{\phi})] = \mathbb{E}_{p(\mathbf{x};\boldsymbol{\theta})}[f(\mathbf{x})\nabla_{\boldsymbol{\theta}}\log p(\mathbf{x};\boldsymbol{\theta})] = \frac{1}{N}\sum_{n=1}^{N} f(\hat{\mathbf{x}}^{(n)}) \nabla_{\boldsymbol{\theta}}\log p(\hat{\mathbf{x}}^{(n)};\boldsymbol{\theta}); \quad \hat{\mathbf{x}}^{(n)} \sim p(\mathbf{x};\boldsymbol{\theta})
$$

- Sample N masks from the probability distribution p
- Compute the weighted avg. of the samples where:
	- \bullet weight = derivative of the log prob. of the sample mask
- update the parameters of the selector network using this weighted average

REDUCING VARIANCE

$$
\mathcal{F}(\boldsymbol{\theta}) := \int p(\mathbf{m}; \mathbf{x}, \boldsymbol{\theta}) f(\mathbf{m} \odot \mathbf{x}; \boldsymbol{\phi}) \mathrm{d} \mathbf{x} = \mathbb{E}_{p(\mathbf{m}; \mathbf{x}, \boldsymbol{\theta})} [f(\mathbf{m} \odot \mathbf{x}; \boldsymbol{\phi})]
$$

- Monte Carlo estimators suffer from the problem of high variance
- \bullet Solution: introduce a constant baseline value β

$$
\eta = \mathbb{E}_{p(x;\theta)}[(f(x) - \beta)\nabla_{\theta} \log p(x;\theta)]
$$

CONCLUSION

- Prefer simple models for better interpretability
- Regularisation for enforcing sparsity in the parameter space
- Feature selection for enforcing sparsity in the feature space
- Instance-wise feature selection selects different features based on different instances
- Selector and predictor architecture for instance-wise feature selection
- Optimisation using without explanation data requires tricks like Monte-Carlo sampling with gradients

REFERENCES

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