Probabilistic modelling for NLP powered by deep learning

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Outline

1. Deep generative models
2. Variational inference
3. Variational auto-encoder

Problems

Supervised problems

"learn a distribution over observed data"

- sentences in natural language
- images, . . .

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Supervised problems

"learn a distribution over observed data"

- sentences in natural language
- images, ...

Unsupervised problems

"learn a distribution over observed and unobserved data"

- sentences in natural language + parse trees
- images + bounding boxes, ...

Supervised problems

We have data $x^{(1)}, \dots, x^{(N)}$ e.g.

- sentences, images, ...

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- with **known** probability (mass/density) function e.g.

$$\underbrace{X \sim \mathrm{Cat}(\pi_1, \ldots, \pi_K)}_{\text{e.g. nationality}} \qquad \text{or} \qquad \underbrace{X \sim \mathcal{N}(\mu, \sigma^2)}_{\text{e.g. height}}$$

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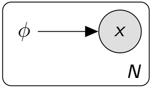
estimate parameters that assign maximum likelihood to observations

Multiple problems, same language



(Conditional) Density estimation

	Side information (ϕ)	Observation (x)
Parsing	a sentence	parse tree
Translation	a sentence in French	translation in English
Captioning	an image	caption in English
Entailment	a text and hypothesis	entailment relation

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Have neural networks predict parameters of our probabilistic model

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$$X|\phi \sim \mathrm{Cat}(\pi_w(\phi)) \qquad \text{or} \qquad X|\phi \sim \mathcal{N}(\mu_w(\phi), \sigma_w(\phi)^2)$$

and proceed to estimate parameters w of the NNs

NN as efficient parametrisation

From the statistical point of view NNs do not generate data

- they parametrise distributions that *by assumption* govern data
- compact and efficient way to map from complex side information to parameter space

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Prediction is done by a decision rule outside the statistical model

- e.g. beam search

MLE via gradient-based optimisation

The probability of an observation $X = x$ is given by some differentiable probability function $p(x)$

- the parameters of which are predicted by f_w *(also differentiable)*

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Example: K classes

$$p(x) = \mathrm{Cat}(X = x | \underbrace{\pi_1^K := f_w(\phi)}_{\text{class probabilities}}) = \prod_{i=1}^{K} \pi_i^{[x=i]}$$

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Given a dataset of i.i.d. observations, SGD gives us a local optimum of the log-likelihood

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Maximum likelihood estimation

- tells you which loss to optimise
  (i.e. negative log-likelihood)

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- chain rule of derivatives: "give me a tractable forward pass and I will give you gradients"

DL in NLP recipe

Maximum likelihood estimation

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  (i.e. negative log-likelihood)

Automatic differentiation (*backprop*)

- chain rule of derivatives: “give me a tractable forward pass and I will give you gradients”

Stochastic optimisation powered by backprop

- general purpose gradient-based optimisers

Tractability is central

Likelihood gives us a differentiable objective to optimise for

- but we need to stick with tractable likelihood functions

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Unsupervised problems

assessing the likelihood requires marginalisation of latent variables

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- too many forward passes

$$p(x) = \sum_{c=1}^{K} \mathrm{Cat}(c|\pi_1, \ldots, \pi_K) \underbrace{\mathcal{N}(x|\mu_w(c), \sigma_w(c)^2)}_{\text{forward pass}}$$

When do we have intractable likelihood?

Unsupervised problems

assessing the likelihood requires marginalisation of latent variables

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- even infinitely many

$$p(x) = \int \mathcal{N}(z|0, I) \underbrace{\mathrm{Cat}(x|\pi_w(z))}_{\text{forward pass}} \mathrm{d}z$$

Deep generative models

Joint distribution with **deep observation model**

$$p_\theta(x, z) = \underbrace{p(z)}_{\text{prior}} \underbrace{p_\theta(x|z)}_{\text{likelihood}}$$

mapping from latent variable z to $p(x|z)$ is a NN with parameters θ

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Marginal likelihood (or evidence)

$$p_\theta(x) = \int p_\theta(x, z) \,\mathrm{d}z = \int p(z)p_\theta(x|z) \,\mathrm{d}z$$

intractable in general

Gradient

Exact gradient is intractable

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$$\begin{aligned}\nabla_\theta \log p_\theta(x) &= \nabla_\theta \log \underbrace{\int p_\theta(x,z)\,\mathrm{d}z}_{\text{marginal}} \\ &= \underbrace{\frac{1}{\int p_\theta(x,z)\,\mathrm{d}z} \int \nabla_\theta p_\theta(x,z)\,\mathrm{d}z}_{\text{chain rule}}\end{aligned}$$

Gradient

Exact gradient is intractable

$$
\begin{aligned}
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&= \frac{1}{p_\theta(x)} \int \underbrace{p_\theta(x,z) \nabla_\theta \log p_\theta(x,z)}_{\text{log-identity for derivatives}}\,\mathrm{d}z
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&= \mathbb{E}_{p_\theta(z|x)}\left[\nabla_\theta \log p_\theta(x,Z)\right]
\end{aligned}$$

MC estimate of gradient requires sampling from posterior

$$p_\theta(z|x) = \frac{p(z)p_\theta(x|z)}{\color{red}{p_\theta(x)}}$$

unavailable due to the intractability of the marginal

Summary

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- But we cannot use backprop for parameter estimation

We need approximate inference techniques!

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The Basic Problem

The marginal likelihood

$$p(x) = \int p(x, z)\mathrm{d}z$$

is generally **intractable**, which prevents us from computing quantities that depend on the posterior $p(z|x)$

- e.g. gradients in MLE
- e.g. predictive distribution in Bayesian modelling

Strategy

Accept that $p(z|x)$ is not computable.

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Accept that $p(z|x)$ is not computable.

- approximate it by an auxiliary distribution $q(z|x)$ that is computable
- choose $q(z|x)$ as close as possible to $p(z|x)$ to obtain a faithful approximation

Evidence lowerbound

$$\log p(x) = \log \int p(x, z)\mathrm{d}z$$

Evidence lowerbound

$$\begin{aligned}\log p(x) &= \log \int p(x,z)\mathrm{d}z \\ &= \log \int q(z|x)\frac{p(x,z)}{q(z|x)}\mathrm{d}z\end{aligned}$$

Evidence lowerbound

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&= \log \int q(z|x)\frac{p(x,z)}{q(z|x)}\mathrm{d}z \\
&= \log\left(\mathbb{E}_{q(z|x)}\left[\frac{p(x,z)}{q(z|x)}\right]\right)
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Evidence lowerbound

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\log p(x) &= \log \int p(x,z)\mathrm{d}z \\
&= \log \int {\color{red} q(z|x)} \frac{p(x,z)}{\color{red} q(z|x)} \mathrm{d}z \\
&= \log \left(\mathbb{E}_{q(z|x)} \left[\frac{p(x,z)}{q(z|x)} \right] \right) \\
&\geq \underbrace{\mathbb{E}_{q(z|x)} \left[\log \frac{p(x,z)}{q(z|x)} \right]}_{\text{ELBO}}
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&\geq \underbrace{\mathbb{E}_{q(z|x)}\left[\log \frac{p(x, z)}{q(z|x)}\right]}_{\text{ELBO}} \\
&= \mathbb{E}_{q(z|x)}\left[\log p(x, z)\right] + \mathbb{H}\left(q(z|x)\right)
\end{aligned}
$$

An approximate posterior

$$\log p(x) \geq \underbrace{\mathbb{E}_{q(z|x)}\left[\log \frac{p(x,z)}{q(z|x)}\right]}_{\text{ELBO}}$$

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\log p(x) &\geq \underbrace{\mathbb{E}_{q(z|x)}\left[\log \frac{p(x,z)}{q(z|x)}\right]}_{\text{ELBO}} \\
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&= \int q(z|x) \log \frac{p(z|x)}{q(z|x)} \mathrm{d}z + \underbrace{\log p(x)}_{\text{constant}}
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$$

We have derived a lower bound on the log-evidence whose gap is exactly $\operatorname{KL}\left(q(z|x) \mid\mid p(z|x)\right)$.

Variational Inference

Objective

$$\max_{q(z|x)} \mathbb{E}\left[\log p(x, z)\right] + \mathbb{H}\left(q(z|x)\right)$$

- The ELBO is a lower bound on $\log p(x)$

Blei et al. (2016)

Mean field assumption

Suppose we have N latent variables

- assume the posterior factorises as N independent terms
- each with an independent set of parameters

$$q(z_1, \ldots, q_N) = \underbrace{\prod_{i=1}^{N} q_{\lambda_i}(z_i)}_{\text{mean field}}$$

Amortised variational inference

Amortise the cost of inference using NNs

$$q(z_1, \ldots, q_N | x_1, \ldots, x_N) = \prod_{i=1}^{N} q_\lambda(z_i | x_i)$$

with a shared set of parameters

- e.g. $Z|x \sim \mathcal{N}(\underbrace{\mu_\lambda(x), \sigma_\lambda(x)^2}_{\text{inference network}})$

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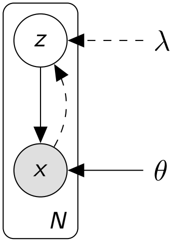
Variational auto-encoder

Generative model with NN likelihood



- complex (non-linear) observation model $p_\theta(x|z)$
- complex (non-linear) mapping from data to latent variables $q_\lambda(z|x)$

Jointly optimise generative model $p_\theta(x|z)$ and inference model $q_\lambda(z|x)$ under the same objective (ELBO)

Kingma and Welling (2013)

Objective

$$\log p(x) \geq \overbrace{\mathbb{E}_{q_\lambda(z|x)}\left[\log p_\theta(x, z)\right] + \mathbb{H}\left(q_\lambda(z|x)\right)}^{\text{ELBO}}$$

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\end{aligned}
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Parameter estimation

$$
\arg\max_{\theta,\lambda} \; \mathbb{E}_{q_\lambda(z|x)}\left[\log p_\theta(x|z)\right] - \mathrm{KL}\left(q_\lambda(z|x) \,||\, p(z)\right)
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Parameter estimation

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- assume $\mathrm{KL}\left(q_\lambda(z|x) \mid\mid p(z)\right)$ analytical
  true for exponential families

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Parameter estimation

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- assume $\mathrm{KL}\left(q_\lambda(z|x) \mid\mid p(z)\right)$ analytical
  true for exponential families
- approximate $\mathbb{E}_{q_\lambda(z|x)}\left[\log p_\theta(x|z)\right]$ by sampling
  true because we design $q_\lambda(z|x)$ to be simple

Generative Network Gradient

$$\frac{\partial}{\partial \theta}\left(\mathbb{E}_{q_\lambda(z|x)}\left[\log p_\theta(x|z)\right] - \overbrace{\mathrm{KL}\left(q_\lambda(z|x) \mid\mid p(z)\right)}^{\text{constant wrt } \theta}\right)$$

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$$= \mathbb{E}_{q_\lambda(z|x)}\left[\frac{\partial}{\partial\theta}\log p_\theta(x|z)\right]$$

$$\overset{\text{MC}}{\approx} \frac{1}{S}\sum_{i=1}^{S}\frac{\partial}{\partial\theta}\log p_\theta(x|z_i)$$

Generative Network Gradient

$$\frac{\partial}{\partial\theta}\left(\mathbb{E}_{q_\lambda(z|x)}\left[\log p_\theta(x|z)\right] - \overbrace{\mathrm{KL}\left(q_\lambda(z|x)\;||\;p(z)\right)}^{\text{constant wrt } \theta}\right)$$

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$$\overset{\text{MC}}{\approx} \frac{1}{S}\sum_{i=1}^{S}\frac{\partial}{\partial\theta}\log p_\theta(x|z_i)$$

Note: $q_\lambda(z|x)$ does not depend on θ.

Inference Network Gradient

$$\frac{\partial}{\partial \lambda}\left(\mathbb{E}_{q_\lambda(z|x)}\left[\log p_\theta(x|z)\right] - \overbrace{\mathrm{KL}\left(q_\lambda(z|x) \mid\mid p(z)\right)}^{\text{analytical}}\right)$$

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The first term again requires approximation by sampling, but there is a problem

Inference Network Gradient

$$\begin{aligned}
&\frac{\partial}{\partial \lambda}\mathbb{E}_{q_\lambda(z|x)}\left[\log p_\theta(x|z)\right] \\
&= \frac{\partial}{\partial \lambda}\int q_\lambda(z|x)\log p_\theta(x|z)\mathrm{d}z \\
&= \underbrace{\int \frac{\partial}{\partial \lambda}(q_\lambda(z|x))\log p_\theta(x|z)\,\mathrm{d}z}_{\text{not an expectation}}
\end{aligned}$$

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- MC estimator is non-differentiable: cannot sample first

Inference Network Gradient

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\end{aligned}
$$

- MC estimator is non-differentiable: cannot sample first
- Differentiating the expression does not yield an expectation: cannot approximate via MC

Reparametrisation

Find a transformation $h : z \mapsto \epsilon$ such that
ϵ does not depend on λ

- $h(z, \lambda)$ needs to be invertible
- $h(z, \lambda)$ needs to be differentiable

(Kingma and Welling, 2013; Rezende et al., 2014; Titsias and Lázaro-Gredilla, 2014)

Reparametrisation

Find a transformation $h : z \mapsto \epsilon$ such that

ϵ does not depend on λ

- $h(z, \lambda)$ needs to be invertible
- $h(z, \lambda)$ needs to be differentiable

Invertibility implies

- $h(z, \lambda) = \epsilon$
- $h^{-1}(\epsilon, \lambda) = z$

(Kingma and Welling, 2013; Rezende et al., 2014; Titsias and Lázaro-Gredilla, 2014)

Gaussian Transformation

If $Z \sim \mathcal{N}(\mu_\lambda(x), \sigma_\lambda(x)^2)$ then

$$h(z, \lambda) = \frac{z - \mu_\lambda(x)}{\sigma_\lambda(x)} = \epsilon \sim \mathcal{N}(0, \mathrm{I})$$

$$h^{-1}(\epsilon, \lambda) = \mu_\lambda(x) + \sigma_\lambda(x) \odot \epsilon \quad \epsilon \sim \mathcal{N}(0, \mathrm{I})$$

Inference Network – Reparametrised Gradient

$$= \frac{\partial}{\partial \lambda} \int q_\lambda(z|x) \log p_\theta(x|z) \, \mathrm{d}z$$

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$$= \int q(\epsilon) \frac{\partial}{\partial \lambda} \left[\log p_\theta(x|\overbrace{h^{-1}(\epsilon, \lambda)}^{=z}) \right] \mathrm{d}\epsilon$$

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$$= \int q(\epsilon) \frac{\partial}{\partial \lambda} \left[\log p_\theta(x| \overbrace{h^{-1}(\epsilon, \lambda)}^{=z}) \right] \mathrm{d}\epsilon$$

$$= \int q(\epsilon) \underbrace{\frac{\partial}{\partial z} \log p_\theta(x| \overbrace{h^{-1}(\epsilon, \lambda)}^{=z}) \times \frac{\partial}{\partial \lambda} h^{-1}(\epsilon, \lambda)}_{\text{chain rule}} \, \mathrm{d}\epsilon$$

Inference Network – Reparametrised Gradient

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$$= \mathbb{E}_{q(\epsilon)} \left[\frac{\partial}{\partial z} \log p_\theta(x| \overbrace{h^{-1}(\epsilon, \lambda)}^{=z}) \times \frac{\partial}{\partial \lambda} h^{-1}(\epsilon, \lambda) \right]$$

Inference Network – Reparametrised Gradient

$$= \mathbb{E}_{q(\epsilon)}\left[\frac{\partial}{\partial z}\log p_\theta(x|\overbrace{h^{-1}(\epsilon,\lambda)}^{=z}) \times \frac{\partial}{\partial \lambda} h^{-1}(\epsilon,\lambda)\right]$$

Inference Network – Reparametrised Gradient

$$= \mathbb{E}_{q(\epsilon)}\left[\frac{\partial}{\partial z}\log p_\theta(x|\overbrace{h^{-1}(\epsilon,\lambda)}^{=z}) \times \frac{\partial}{\partial \lambda} h^{-1}(\epsilon,\lambda)\right]$$

$$\overset{\text{MC}}{\approx} \frac{1}{S}\sum_{i=1}^{S} \underbrace{\frac{\partial}{\partial z}\log p_\theta(x|\overbrace{h^{-1}(\epsilon,\lambda)}^{=z}) \times \frac{\partial}{\partial \lambda} h^{-1}(\epsilon,\lambda)}_{\text{backprop's job}}$$

Gaussian KL

ELBO

$$\mathbb{E}_{q_\lambda(z|x)}\left[\log p_\theta(x|z)\right] - \mathrm{KL}\left(q_\lambda(z|x) \mid\mid p(z)\right)$$

Gaussian KL

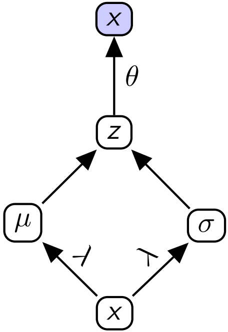
ELBO

$$\mathbb{E}_{q_\lambda(z|x)}\left[\log p_\theta(x|z)\right] - \mathrm{KL}\left(q_\lambda(z|x) \mid\mid p(z)\right)$$

Analytical computation of $-\mathrm{KL}\left(q_\lambda(z|x) \mid\mid p(z)\right)$:

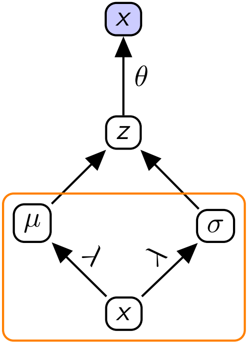
$$\frac{1}{2}\sum_{i=1}^{d}\left(1 + \log\left(\sigma_i^2\right) - \mu_i^2 - \sigma_i^2\right)$$

Computation Graph



Computation Graph

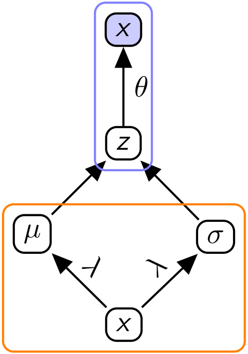
inference model



Computation Graph

generative model

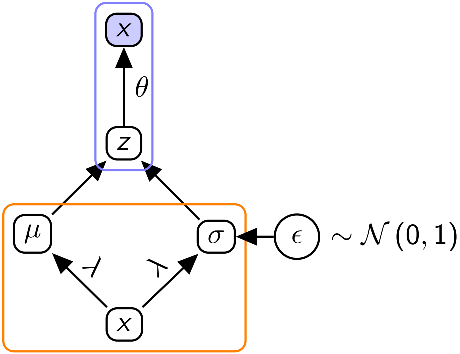
inference model



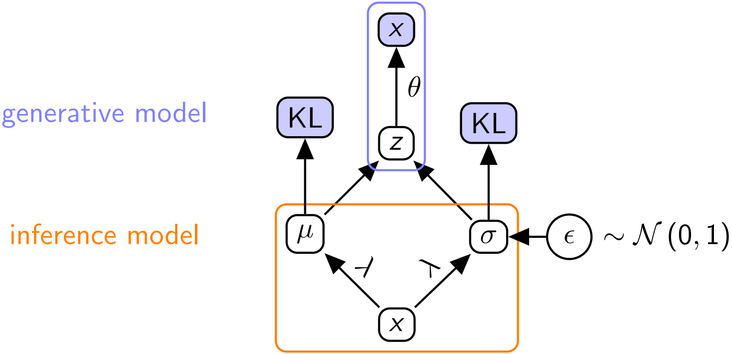
Computation Graph

generative model

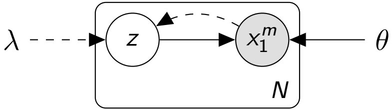
inference model



Computation Graph



Example



Generative model

- $Z \sim \mathcal{N}(0, I)$
- $X_i | z, x_{<i} \sim \text{Cat}(f_\theta(z, x_{<i}))$

Inference model

- $Z \sim \mathcal{N}(\mu_\lambda(x_1^m), \sigma_\lambda(x_1^m)^2)$

Bowman et al. (2016)

VAEs – Summary

Advantages

- Backprop training
- Easy to implement
- Posterior inference possible
- One objective for both NNs

VAEs – Summary

Advantages

- Backprop training
- Easy to implement
- Posterior inference possible
- One objective for both NNs

Drawbacks

- Discrete latent variables are difficult
- Optimisation may be difficult with several latent variables
- Location-scale families only
  but see Ruiz et al. (2016) and Kucukelbir et al. (2017)

Summary

Deep learning in NLP

- task-driven feature extraction
- models with more realistic assumptions

Probabilistic modelling

- better (or at least more explicit) statistical assumptions
- compact models
- semi-supervised learning

Literature I

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