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Rapid Prototyping of Probabilistic Models using Stochastic Variational Inference

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Rapid Prototyping

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- In **data analysis** we often have to develop new models
- This can be a lengthy process
  - We need to derive appropriate inference
  - Often cumbersome implementation which changes regularly
- **Rapid prototyping** is used to answer similar problems in manufacturing
  - "Quick fabrication of scale models of a physical part"
  - Probabilistic programming can be used for rapid prototyping in machine learning

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Today I'm going to argue that Stochastic Variational Inference (SVI) can be used for rapid prototyping as well, with several advantages over probabilistic programming.

Rapid Prototyping

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- SVI is not usually considered as means of speeding-up development
- But this new inference technique allows us to **simplify the derivations** for a large class of models
  - With this we can take advantage of **effective symbolic differentiation**
  - Models are often mathematically **too cumbersome otherwise**
- Similar principles have been used for **rapid model prototyping in deep learning** for NLP for quite some time [Socher, Ng, and Manning 2010, 2011, 2012]

What is SVI?

- SVI is simply **variational inference** used with **noisy gradients** – we thus replace the optimisation with stochastic optimisation
- Variational inference
  - We approximate the posterior of the latent variables with distributions from a tractable family ($q(X)$ for example)

Example model: $X \to Y$

$$\log P(Y) \geq \int q(X) \log \frac{P(Y|X)P(X)}{q(X)} = E_q[\log P(Y|X)] - KL(q||P)$$

What is SVI?

- Stochastic variational inference
  - Often used to speed-up inference using **mini-batches**

$$\log P(Y) \geq \frac{N}{|S|} \sum_{i \in S} E_q[\log P(Y_i | X_i)] - KL(q || P)$$

summing over random subsets of the data points

  - But can also be used to **approximate integrals** through Monte Carlo integration [Kingma and Welling 2014, Rezende et al. 2014, Titsias and Lazaro-Gredilla 2014]

$$E_q[\log P(Y|X)] \approx \frac{1}{K} \sum_{i=1}^{K} \log P(Y|X_i), \; X_i \sim q(X)$$

summing over samples from the approximating distribution

  - Optimising these objectives relies on non-deterministic gradients

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Stochastic optimisation

- Using gradient descent with noisy gradients and decreasing learning-rates, we are guaranteed to converge to an optimum

$$\theta_{t+1} = \theta_t + \alpha f'(\theta_t)$$

- Learning-rates (α) are hard to tune...
  - Use learning-rate free optimisation (again, from deep learning)
  - AdaGrad [Duchi et. al 2011], AdaDelta [Zeiler 2012]
  - RMSPROP [Tieleman and Hinton 2012, Lecture 6.5, COURSERA: Neural Networks for Machine Learning]

$$\theta_{t+1} = \theta_t + \frac{\alpha}{\sqrt{r_t}} f'(\theta_t); \; r_t = (1-\gamma) f'(\theta)^2 + \gamma r_{t-1}$$

and increase α times $1+\epsilon$ if the last two grads' directions agree

  - These have been compared to each other and others *empirically* in a variety of settings in [Schaul 2014]

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Rapid Prototyping with SVI

With **Monte Carlo integration** we can greatly simplify model and inference description

Example model: X $\rightarrow$ Y

Lower bound:

1. Simulate $X_i \sim q(X)$ for $i \leq K$
2. Evaluate $P(Y|X_i)$
3. Return $\frac{1}{K}\sum_{i=1}^{K} \log P(Y|X_i) - KL(q||P)$

Objective:

$$q_{opt} = \arg\max_{q(X)} \frac{1}{K}\sum_{i=1}^{K} \log P(Y|X_i) - KL(q||P)$$

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Objective:

$$q_{opt} = \arg\max_{q(X)} \frac{1}{K} \sum_{i=1}^{K} \log P(Y|X_i) - KL(q||P)$$

Symbolic differentiation is straight-forward in this representation:

$$\frac{\partial}{\partial\theta} \log P(Y|X), \ \frac{\partial}{\partial\theta} KL$$

are easy to compute for a large class of models [Titsias and Lazaro-Gredilla 2014]

Examples: Bayesian logistic regression, variable selection, Gaussian process (GP) hyper-parameter estimation, and more [Titsias and Lazaro-Gredilla 2014]

Example: Bayesian logistic regression

Given dataset with $\mathbf{x}_i \in \mathbb{R}^d$ and $y_i \in \{0, 1\}$ for $n \leq N$, we define

$$P(Y|X, \eta) = \prod_{i=1}^{N} \sigma(y_i \mathbf{x}_i^T \eta)$$

for some vector of weights η with prior $P(\eta) = \mathcal{N}(0, I_d)$.
Define

$$q(\eta|\theta = \{\mu, C\}) = \mathcal{N}(\eta; \mu, CC^T)$$

Symbolically differentiate and optimise wrt

$$\frac{\partial}{\partial\theta} \log\big(\prod_{i=1}^{N} \sigma(y_i \mathbf{x}_i^T \eta)\big), \ \frac{\partial}{\partial\theta} KL$$

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Non-linear density estimation of categorical data (work in progress with Yutian Chen)

Model (using sparse GP with M inducing inputs / outputs Z and U):

$$X \sim \mathcal{N}(0, I)$$
$$(F_K, U_K) \sim GP(X, Z)$$
$$Y \sim Softmax(F_1, ..., F_K)$$

Approximating distributions: $q(X, F, U) = q(X)q(U)p(F|X, U)$, defining $q(x_n) = \mathcal{N}(m_n, s_n^2)$ and $q(u_k) = \mathcal{N}(\mu_k, CC^T)$

We have (with $\epsilon. \sim \mathcal{N}(0, I)$):

$$x_n = m_n + s_n \epsilon_n$$
$$u_k = \mu_k + C\epsilon_k$$
$$f_{nk} = K_{nM}K_{MM}^{-1}u_k + \sqrt{K_{nn} - K_{nM}K_{MM}^{-1}K_{Mn}}\epsilon_{nk}$$
$$y_n = Softmax(f_{n1}, ..., f_{nK})$$

- Original approach took half a year to develop –
  - Deriving variational inference
  - Researching appropriate bound in the statistics literature
  - Derivations for the model

$$\mathcal{L} = -\sum_{n=1}^{N} \mathrm{KL}(q(\mathbf{x}_n) \| p(\mathbf{x}_n))$$

$$+ \sum_{d=1}^{D} \left\{ -\frac{1}{2} \mathbf{Tr}[(I_K \otimes \mathbf{K}_{d,MM}^{-1})(\mathbf{\Sigma}_d + \hat{\boldsymbol{\mu}}_d \hat{\boldsymbol{\mu}}_d^T)] + \frac{MK}{2} + \frac{1}{2} \log |\mathbf{\Sigma}_d| - \frac{1}{2} \log |\mathbf{K}_{d,MM}| \right\}$$

$$+ \sum_{d=1}^{D} \sum_{n=1}^{N} \left\{ -\frac{1}{2} \mathbf{Tr} \left[\left(\mathbf{A}_d \otimes (\mathbf{K}_{d,MM}^{-1} \langle \mathbf{K}_{d,Mn} \mathbf{K}_{d,nM} \rangle_{\mathbf{x}_n} \mathbf{K}_{d,MM}^{-1}) \right) (\mathbf{\Sigma}_d + \hat{\boldsymbol{\mu}}_d \hat{\boldsymbol{\mu}}_d^T) \right] \right.$$

$$+ [(\mathbf{y}_{nd} + \mathbf{b}_{nd})^T \otimes (\langle \mathbf{K}_{d,nM} \rangle_{\mathbf{x}_n} \mathbf{K}_{d,MM}^{-1})] \hat{\boldsymbol{\mu}}_d - c_{nd} - \frac{1}{2} \mathbf{Tr}[\mathbf{A}_d \langle \mathbf{K}_{d,nn} \rangle_{\mathbf{x}_n}] + \frac{1}{2} \mathbf{Tr}(\mathbf{A}_d) \mathbf{Tr}(\mathbf{K}$$

$$= -\sum_{n=1}^{N} \mathrm{KL}(q(\mathbf{x}_n) \| p(\mathbf{x}_n))$$

$$+ \sum^{D} \left\{ -\frac{1}{2} \mathbf{Tr}[(I_K \otimes \mathbf{K}_{MM}^{-1})(\mathbf{\Sigma} + \hat{\boldsymbol{\mu}} \hat{\boldsymbol{\mu}}^T)] + \frac{MK}{2} + \frac{1}{2} \log |\mathbf{\Sigma}| - \frac{1}{2} \log |\mathbf{K}_{MM}| \right.$$

  - Implementation (hundreds of lines of python code)

- New approach –
  - Derivations took a day
  - Programming took a day (15 lines of Python)

Concrete example

- Original approach took half a year to develop –
  - Deriving variational inference
  - Researching appropriate bound in the statistics literature
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```
print 'Building model...'
X = m + T.exp(s) * eps_NQ
U = mu + T.tril(L).dot(eps_MK)

dist_ZZ = T.sum(((T.reshape(Z, (M, 1, Q)) - Z) / ard)**2, 2)
dist_ZX = T.sum(((T.reshape(Z, (M, 1, Q)) - X) / ard)**2, 2)
Kmm = sf2 * T.exp(-dist_ZZ / 2.0)
Kmn = sf2 * T.exp(-dist_ZX / 2.0)
Knn = sf2

KmmInv = sT.matrix_inverse(Kmm)
A = KmmInv.dot(Kmn)
B = Knn - T.sum(Kmn * KmmInv.dot(Kmn), 0)

F = A.T.dot(U) + B[:, None]**0.5 * eps_NK
S = T.nnet.softmax(F)
```

Disadvantages of this approach

- Studying how symbolic differentiation works is important though –
  - Careless implementation can take long to run
  - But careful implementation (together with mini batches) can actually scale well!
- Only suitable when variational inference is; As usual in variational inference depends on the family of approximating distributions
- We can have large variance in the approximate integration
  - Either use more samples (slower to run),
  - Or use variance reduction techniques [Wang, Chen, Smola, and Xing 2013]

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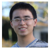
Also thanks to Yutian Chen , Shakir Mohamed , and Richard Socher