Marrying Graphical Models & Deep Learning

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Overview:

- Machine Learning as Computational Statistics
- Graphical Models:
 - Bayes nets
 - MRFs
 - Latent variable models
- Inference:
 - Variational inference
 - MCMC
- Learning:
 - EM
 - Amortized EM
 - Variational autoencoder

- Generative versus discriminative modeling
- Deep Learning:
 - CNN
 - Dropout
- Bayesian inference
 - Bayesian deep models
 - Compression

ML as Statistics

- Data: $\{X_1, ..., X_n, Y_1, ..., Y_n\} \sim P(X_1, ..., X_n, Y_1, ..., Y_n)$
- Optimize objective:
 - maximize log likelihood:

minimize loss:

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$$\max_{\Theta} \log P(X_1, ..., X_n | \Theta) \qquad (unsupervised)$$

$$\max_{\Theta} \log P(Y_1, ..., Y_n | X_1, ..., X_n, \Theta) \qquad (supervised)$$

$$\min_{\Theta} \sum_i Loss(Y_i, \hat{Y}(X_i, \Theta)) \qquad (supervised)$$

- *ML is more than an optimization problem: it's a statistical inference problem.*
 - E.g.: you should not optimize parameters more precisely than the scale at which the MLE fluctuates under resampling the data: $\Theta_{mle}(X,Y) \approx \Theta'_{mle}(X',Y')$, or risk overfitting.

Bias Variance Tradeoff





 $Y = f(X) + \epsilon \qquad \epsilon \sim \mathcal{N}(0, \sigma_{\epsilon}).$ $Err(x) = E\left[(Y - \hat{f}(x))^{2}\right]$ $Err(x) = \left(E[\hat{f}(x)] - f(x)\right)^{2} + E\left[\left(\hat{f}(x) - E[\hat{f}(x)]\right)^{2}\right] + \sigma_{e}^{2}$ $Err(x) = \text{Bias}^{2} + \text{Variance} + \text{Irreducible Error}$

Model Complexity

Graphical Models

- A graphical representation to concisely represent (conditional) independence relations between variables.
- There is a one-to-one correspondence between the dependencies implied by the graph and the probabilistic model.
- E.g. Bayes Nets



P(all) = P(traffic-jam | rush-hour, bad-weather, accident) x P(sirens | accident) x P(accident | bad-weather) x P(bad-weather) x P(rush-hour)

P(rush-hour) independent P(bad-weather) $\leftarrow \rightarrow$ sum_{traffic-jam,sirens,accident) P(all) = P(rush-hour) P(bad-weather)



Rush-hour independent of bad-weather

Bayes ball algorithm

An undirected path is active if a Bayes ball travelling along it never encounters the "stop" symbol: \longrightarrow



If there are no active paths from X to Y when $\{Z_1, \ldots, Z_k\}$ are shaded, then $X \perp \!\!\!\perp Y \mid \{Z_1, \ldots, Z_k\}.$

CS188: Computational Models of Human Behavior

Source:

INTRODUCTION TO GRAPHICAL MODELS SLIDE CREDITS: KEVIN MURPHY, MARK PASHKIN, ZOUBIN GHAHRAMANI AND JEFF BILMES

Markov Random Fields



A independent B given C (for independence, all paths must be blocked)

Probability distribution:
$$P(X) = \frac{\prod_{c} \Psi_{c}(X_{c})}{Z}$$

 $\Psi_c(X_c)$: maximal clique = largest completely connected subgraphs

Hammersley-Clifford Theorem: if P>0 all x, then all (conditional) independencies in P match those of the graph.

Latent Variable Models

• Introducing latent (unobserved) variables will dramatically increase the capacity of a model.



$$P(X) = \sum_{Z} P(X|Z)P(Z)$$

• Problem: P(Z|X) is intractable for most nontrivial models

Approximate Inference



Independence Samplers & MCMC





Sample from g and suppress samples with low $p(\theta | X)$ e.g. a) Rejection Sampling b) Importance Sampling

- Does not scale to high dimensions

Markov Chain Monte Carlo



- Make steps by perturbing previous sample
- Probability of visiting a state is equal to $P(\theta | X)$

Sampling 101 – What is MCMC?



Sampling 101 – Metropolis-Hastings



Approximate MCMC



Decreasing ϵ

Minimizing Risk



Stochastic Gradient Langevin Dynamics

Welling & Teh 2011

Gradient AscentLangevin Dynamics
$$\Delta \theta_t = \frac{\epsilon}{2} \left(\nabla \log p(\theta_t) + \sum_{i=1}^N \nabla \log p(x_i; \theta_t) \right)$$
$$\Delta \theta_t = \frac{\epsilon}{2} \left(\nabla \log p(\theta_t) + \sum_{i=1}^N \nabla \log p(x_i; \theta_t) \right) + \mathbb{N}(0, \epsilon)$$
$$\downarrow$$
Metropolis-Hastings Accept Step

Stochastic Gradient AscentStochastic Gradient Langevin Dynamics
$$\Delta \theta_t = \frac{\epsilon_t}{2} \left(\nabla \log p(\theta_t) + \frac{N}{n} \sum_{i=1}^n \nabla \log p(x_{t_i}; \theta_t) \right)$$
 $\Delta \theta_t = \frac{\epsilon_t}{2} \left(\nabla \log p(\theta_t) + \frac{N}{n} \sum_{i=1}^n \nabla \log p(x_{t_i}; \theta_t) \right) + \mathbb{N}(0, \epsilon_t)$ $\sum_{t=1}^{\infty} \epsilon_t = \infty$ $\sum_{t=1}^{\infty} \epsilon_t^2 < \infty$ e.g. $\epsilon_t = \frac{a}{(b+t)^{\gamma}}$ Metropolis-Hastings Accept Step

Demo: Stochastic Gradient LD



A Closer Look ...



A Closer Look ...



Demo SGLD: large stepsize



Demo SGLD: small stepsize



Variational Inference

- Choose tractable family of distributions (e.g. Gaussian, discrete)
- Minimize over Q: KL[Q(Z|X)||P(Z||X)]
- Equivalent to maximize over Φ : $\sum_Z Q(Z|X, \Phi) \left(\log P(X|Z, \Theta) P(Z) \log Q(Z|X, \Phi)\right)$



Learning: Expectation Maximization KL[Q(Z|X)||P(Z||X)] $\log P(X|\Theta) =$ Gap: $\log \sum P(X|Z,\Theta)P(Z) \ge$ Bound $B(\Theta, \Phi)$ $\sum Q(Z|X,\Phi) \left(\log P(X|Z,\Theta)P(Z) - \log Q(Z|X,\Phi)\right)$ $\underset{\Phi}{\arg\max} \ B(\Theta, \Phi)$ E-step: (variational inference) $\arg\max_{\Theta} B(\Theta, \Phi)$ M-step: (approximate learning)

Amortized Inference



 Bij making q(z|x) a function of x and sharing parameters φ , we can do very fast inference at test time (i.e. avoid iterative optimization of q_{test}(z))

Deep NN as a glorified conditional distribution





The "Deepify" Operator

- Find a graphical model with conditional distributions and replace those with a deep NN.
- Logistic regression \rightarrow deep NN.
- "deep survival analysis". Cox's proportional hazard function:

$$\lambda_i(t|\mathbf{x}_i) = \lambda_0(t) \exp\{\mathbf{x}_i' oldsymbol{eta}\}$$
 . Replace with deep NN!

 Latent variable model: replace generative and recognition models with deep NNs: → "Variational Autoencoder" (VAE).

Variational Autoencoder



Deep Generative Model: The Variational Auto-Encoder



Stochastic Variational Bayesian Inference

$$B(Q) = \sum_{Z} Q(Z|X, \Phi) (\log P(X|Z, \Theta) + \log P(Z) - \log Q(Z|X, \Phi))$$

$$\nabla_{\Phi} B(Q) = \sum_{Z} Q(Z|X, \Phi) \nabla_{\Phi} \log Q(Z|X, \Phi) (\log P(X|Z, \Theta) + \log P(Z) - \log Q(Z|X, \Phi))$$

$$\sum_{Z \in \mathcal{A}} Subsample \text{ mini-batch } X$$

$$\nabla_{\Phi} B(Q) = \frac{1}{N} \frac{1}{S} \sum_{i=1}^{N} \sum_{s=1}^{S} \nabla_{\Phi} \log Q(Z_{is} | X_i, \Phi) (\log P(X_i | Z_{is}, \Theta) + \log P(Z_{is}) - \log Q(Z_{is} | X_i, \Phi))$$

$$\mathsf{very high variance}$$

Reducing the Variance: The Reparametrization Trick

Kingma 2013, Bengio 2013, Kingma & Welling 2014



• Example:
$$\nabla_{\mu} \int dz \mathcal{N}_{z}(\mu, \sigma) z$$

 $= \frac{1}{S} \sum_{s} z_{s}(z_{s} - \mu) / \sigma^{2}, \quad z_{s} \sim \mathcal{N}_{z}(\mu, \sigma)$
or $\frac{1}{S} \sum_{s} 1, \quad \epsilon_{s} \sim \mathcal{N}_{\epsilon}(0, 1), \quad z = \mu + \sigma \epsilon$

Semi-Supervised VAE I

D.P. Kingma, D.J. Rezende, S. Mohamed, M. Welling, NIPS 2014



Discriminative or Generative? -Deep Learning Variational Auto-Encoder -Bayesian Networks -Kernel Methods -Probabilistic Programs -Random Forests -Simulator Models -Boosting

- Advantages discriminative models:
 - Flexible map from input to target (low bias)
 - Efficient training algorithms available
 - Solve the problem you are evaluating on.
 - Very successful and accurate!

- Advantages generative models:
 - Inject expert knowledge
 - Model causal relations
 - Interpretable
 - Data efficient
 - More robust to domain shift
 - Facilitate un/semi-supervised learning

Big N vs. Small N?



Combining Generative and Discriminative Models



Deep Convolutional Networks

• Input dimensions have "topology": (1D, speech, 2D image, 3D MRI, 2+1D video, 4D fMRI)

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Forward: Filter, subsample, filter, nonlinearity, subsample,, classify



Backward: backpropagation (propagate error signal backward)

Dropout



Figure 1: Dropout Neural Net Model. Left: A standard neural net with 2 hidden layers. Right: An example of a thinned net produced by applying dropout to the network on the left. Crossed units have been dropped.



Example: Dermatology

Dermatologist-level classification of skin cancer with deep neural networks

Andre Esteva¹*, Brett Kuprel¹*, Roberto A. Novoa^{2,3}, Justin Ko², Susan M. Swetter^{2,4}, Helen M. Blau⁵ & Sebastian Thrun⁶









Beter dan de patholoog

Datzelfde principe heeft Google nu toegepast op de data van het Radboud. Het algoritme werd geprogrammeerd om kankercellen te vinden op de foto's en vervolgens aan het werk gezet. Volgens de onderzoekers haalde het algoritme een score van 89 procent, terwijl een patholoog gemiddeld 73 procent haalt op dezelfde foto's.

Example: Retinopathy

JAMA | Original Investigation | INNOVATIONS IN HEALTH CARE DELIVERY

Development and Validation of a Deep Learning Algorithm for Detection of Diabetic Retinopathy in Retinal Fundus Photographs

Varun Gulshan, PhD; Lily Peng, MD, PhD; Marc Coram, PhD; Martin C. Stumpe, PhD; Derek Wu, BS; Arunachalam Narayanaswamy, PhD; Subhashini Venugopalan, MS; Kasumi Widner, MS; Tom Madams, MEng; Jorge Cuadros, OD, PhD; Ramasamy Kim, OD, DNB; Rajiv Raman, MS, DNB; Philip C. Nelson, BS; Jessica L. Mega, MD, MPH; Dale R. Webster, PhD





What do these Problems have in common?



It's the same CNN in all cases: Inception-v3

So..., CNNs work really well.

However:

- They are way too big
- They consume too much energy
- They use too much memory
- → we need to make them more efficient!



Reasons for Bayesian Deep Learning

- Automatic model selection / pruning
- Automatic regularization
- Realistic prediction uncertainty (important for decision making)





Computer Aided Diagnosis

Autonomous Driving

Example



Increased uncertainty away from data

Bayesian Learning

$$P(X|M) = \int d\Theta \ P(X|\Theta, M)P(\Theta|M) \quad (\text{model evidence})$$

$$P(\Theta|X, M) = \frac{P(X|\Theta, M)P(\Theta|M)}{P(X|M)} \quad (\text{posterior})$$

$$P(x|X, M) = \int d\Theta \ P(x|\Theta, M)P(\Theta|X, M) \quad (\text{prediction})$$

$$P(X) = \sum_{M} P(X|M)P(M) \quad (\text{evidence})$$

$$P(M|X) = \frac{P(X|M)P(M)}{P(X)} \quad (\text{model selection})$$

Variational Bayes

$$\log P(X) \ge \int_{\Theta} d\Theta \ Q(\Theta) \left[\log P(X|\Theta) + \log P(\Theta) - \log Q(\Theta) \right] \equiv B(Q(\Theta)|X)$$

 $= E_{Q(\Theta)}[\log P(X|\Theta)] - KL[Q(\Theta)||P(\Theta)])$

Sparsifying & Compressing CNNs

- DNNs are vastly overparameterized (e.g. distillation, Bucilua et al 2006).
- Interpret variational bound as coding cost for data transmission (minimum description length)
- Idea: learn a soft weight sharing prior, a.k.a. quantize the weights (Nowlan & Hinton 1991, Ullrich et al 2016)

$$E_{Q(\Theta)}[\log P(X|\Theta)] - KL[Q(\Theta)||P(\Theta)])$$

$$(F_{Q(\Theta)}[\log P(X|\Theta)] - KL[Q(\Theta)||P(\Theta)])$$

$$(F_{Q(\Theta)}[\log P(X|\Theta)] - KL[Q(\Theta)||P(\Theta)])$$

$$(F_{Q(\Theta)}[\log P(X|\Theta)] - KL[Q(\Theta)||P(\Theta)])$$

Full Bayesian Deep Learning

The signal in NNs are very robust to noise addition (e.g dropout)



THE PLAN:

- Marginalize out weights for the price of introducing stochastic hidden units.
- Reinterpret stochasticity on hidden units as dropout noise.
- Use sparsity inducing priors to prune weights / hidden units.

Stochastic Variational Bayes

$$B(Q(\Theta)|X) = \int_{\Theta} d\Theta \ Q(\Theta) \left[\log P(X|\Theta) + \log P(\Theta) - \log Q(\Theta)\right]$$

$$\nabla_{\Phi}B = \int_{\Theta} d\Theta \quad Q_{\Phi}(\Theta) \nabla_{\Phi} \log Q_{\Phi}(\Theta) \left[\log P(X|\Theta) + \log P(\Theta) - \log Q_{\Phi}(\Theta)\right]$$
subsample mini-batch X
$$\nabla_{\Phi}B = \frac{1}{S} \sum_{s=1}^{S} \nabla_{\Phi} \log Q_{\Phi}(\Theta_s) \left[\frac{N}{n} \sum_{i=1}^{n} \log P(x_i|\Theta_s) + \log P(\Theta_s) - \log Q_{\Phi}(\Theta_s)\right]$$
very high variance ******

Reparametrization? Yes but not enough: same sample ⊖_s for all data cases X_i in minibatch induces high correlations between data-cases and thus high variance in gradient.

Local Reparametrization

Kingma, Salimans & Welling 2015

 $(P(X|\Theta) \rightarrow P(Y|W,X))$

 $dWQ(W)\log P(Y|X,W) - \operatorname{KL}(Q(W)||P(W))$ compute exactly Reparameterize: $\int dW dF \ Q(W) \ L(Y, \phi(F)) \ I(F - W\phi(B(X))) =$ $dF \ Q(F|B) \ L(Y,\phi(F))$

- Hidden units now become stochastic and correlated.
- We draw different samples F_{is} for different data-cases in the minibatch (and it's much less expensive than resampling all the weights independently per data case)

Conclusion: using this trick we can further reduce variance in the gradients







Conclusion: by using a special form of posterior we simulate dropout noise: i.e. dropout can be understood as variational Bayesian inference with multiplicative noise.

Y Gal, Z Ghahramani 2016, Dropout as a Bayesian approximation: Representing model uncertainty in deep learning

<u>S Wang</u>, <u>C Manning</u>, Fast dropout training

Sparsity Inducing Priors

(Kingma, Salimans, Welling 2015, Mochanov, Ashuka, Vetrov 2017)



$$-D_{KL}(q(w_{ij} | \theta_{ij}, \alpha_{ij}) \parallel p(w_{ij})) \approx$$
$$\approx k_1 \sigma (k_2 + k_3 \log \alpha_{ij})) - 0.5 \log(1 + \alpha_{ij}^{-1}) + C$$
$$k_1 = 0.63576 \quad k_2 = 1.87320 \quad k_3 = 1.48695$$

Learn dropout rate α_{ij} . When $\alpha_{ij} \to \infty$ weight is pruned

Conclusion: we can learn the dropout rates and prune unnecessary weights.

Variational Dropout



Epoch: 0 Compression ratio: 1x Accuracy: 0.113

Animation: Molchanov, D., Ashukha, A. and Vetrov, D.





Animation: Molchanov, D., Ashukha, A. and Vetrov, D.

Node (instead of Weight) Sparsification

(Louizos, Ullrich, Welling, 2017)

Use hierarchical prior:
$$P(W, z) = \prod_{\text{hidden units i}} p(z_i) \prod_{\text{units j outgoing from node i}} P(w_{ij}|z_i)$$

Prior-posterior pair
$$\int_{a_{i}}^{a_{i}} p(\mathbf{W}, \mathbf{z}) \propto \prod_{i}^{A} \frac{1}{|z_i|} \prod_{ij}^{A,B} \mathcal{N}(w_{ij}|0, z_i^2) \prod_{i,j}^{A,B} \mathcal{N}(w_{ij}|z_i\mu_{ij}, z_i^2\sigma_{ij}^2) \prod_{j=1}^{A} \mathcal{N}(z_i|\mu_{z_i}, \sigma_{z_i}^2) \prod_{i,j}^{A,B} \mathcal{N}(w_{ij}|z_i\mu_{ij}, z_i^2\sigma_{ij}^2) \prod_{j=1}^{A} \mathcal{N}(z_i^2|\mu_{z_i}, \sigma_{z_i}^2) \prod_{j=1}^{A,B} \mathcal{N}(w_{ij}|z_i\mu_{ij}, z_i^2\sigma_{ij}^2) \prod_{j=1}^{A} \mathcal{N}(z_j^2|\mu_{z_j}, \sigma_{z_j}^2) \prod_{j=1}^{A,B} \mathcal{N}(w_{ij}|z_i\mu_{ij}, z_i^2\sigma_{ij}^2) \prod_{j=1}^{A} \mathcal{N}(z_j^2|\mu_{z_j}, \sigma_{z_j}^2) \prod_{j=1}^{A,B} \mathcal{N}(w_{ij}|z_j\mu_{ij}, z_j^2\sigma_{ij}^2) \prod_{j=1}^{A} \mathcal{N}(z_j^2|\mu_{z_j}, \sigma_{z_j}^2) \prod_{j=1}^{A} \mathcal{N}(z_j^2|\mu_{z_j}, \sigma_{z_j}^2) \prod_{j=1}^{A} \mathcal{N}(w_{ij}|z_j\mu_{ij}, z_j^2\sigma_{ij}^2) \prod_{j=1}^{A} \mathcal{N}(z_j^2|\mu_{z_j}, \sigma_{z_j}^2) \prod_$$

Conclusion: by using special, hierarchical priors we can prune hidden units instead of individual weights (which is much better for compression).

Preliminary Results

(Louizos, Ullrich, Welling 2017, submitted)

Network & size	Method	Pruned architecture	Bit-precision
LeNet-300-100	Sparse VD	512-114-72	8-11-14
784-300-100	BC-GNJ	278-98-13	8-9-14
	BC-GHS	311-86-14	13-11-10
LeNet-5-Caffe	Sparse VD	14-19-242-131	13-10-8-12
	GD	7-13-208-16	-
20-50-800-500	GL	3-12-192-500	-
	BC-GNJ	8-13-88-13	18-10-7-9
	BC-GHS	5-10-76-16	10-10-14-13
VGG	BC-GNJ	63-64-128-128-245-155-63-	10-10-10-10-8-8-8-
		-26-24-20-14-12-11-11-15	-5-5-5-5-6-7-11
$(2 \times 64) - (2 \times 128) -$	BC-GHS	51-62-125-128-228-129-38-	11-12-9-14-10-8-5-
-(3×256)-(8× 512)		-13-9-6-5-6-6-20	-5-6-6-6-8-11-17-10

Additional Bayesian Bonus: By monitoring posterior fluctuations of weights one can determine their fixed point precision.

			Compression Rates (Error %)		
Model				Fast	Maximum
Original Error %	Method	$\frac{ \mathbf{w}\neq 0 }{ \mathbf{w} }\%$	Pruning	Prediction	Compression
LeNet-300-100	DC	8.0	6 (1.6)	-	40 (1.6)
	DNS	1.8	28* (2.0)	-	-
1.6	SWS	4.3	12* (1.9)	-	64(1.9)
	Sparse VD	2.2	21(1.8)	84(1.8)	113 (1.8)
	BC-GNJ	10.8	9(1.8)	36(1.8)	58(1.8)
	BC-GHS	10.6	9(1.8)	23(1.9)	59(2.0)
LeNet-5-Caffe	DC	8.0	6*(0.7)	-	39(0.7)
	DNS	0.9	55*(0.9)	-	108(0.9)
0.9	SWS	0.5	100*(1.0)	-	162(1.0)
	Sparse VD	0.7	63(1.0)	228(1.0)	365(1.0)
	BC-GNJ	0.9	108(1.0)	361(1.0)	573(1.0)
	BC-GHS	0.6	156(1.0)	419(1.0)	771(1.0)
VGG	BC-GNJ	6.7	14(8.6)	56(8.8)	95(8.6)
8.4	BC-GHS	5.5	18(9.0)	59(9.0)	116(9.2)

- Compression rate of a factor 700x with no loss in accuracy!
- Compression rates for node sparsity are higher because encoding is cheaper.

Conclusions

- Deep learning is a no silver bullet: it is mainly very good at signal processing (auditory, image data)
- Optimization plays an important role in getting good solutions (e.g. reducing variance gradients)
- But... deep learning is more than optimization, it's also statistics!
- DL can be successfully combined with "classical" graphical models (as a glorified conditional distribution)
- Bayesian DL has a elegant interpretation as principled dropout
- Bayesian DL is ideally suited for compression
- There is a lot we do not understand about DL:
 - Why do they not overfit (easy to get 0 training error on data with random labels)
 - Why does SGD regularize so effectively?
 - Strange behavior in the face of adversarial examples
 - Huge over-parameterization (up to 400x)