Log Concave Coupling for Sampling Neural Net Posteriors

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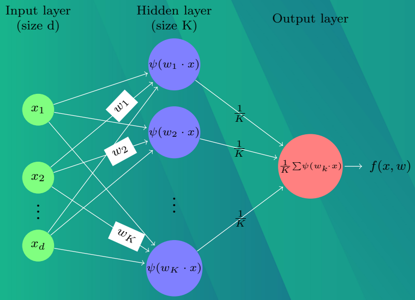
Problem Definition



- Wide single hidden layer neural network
- Outer weights fixed, linear combination of neurons from infinite dictionary
- Train inner weights w not by optimization:

$$w = \text{argmax}_w L(\text{Data}, w)$$

  but via posterior sampling:

$$w \sim p(w|\text{Data}) \propto e^{L(\text{Data}, w)}$$

- Overall fit is posterior mean,

$$\hat{f}(x) = E[f(x, w)|\text{Data}]$$

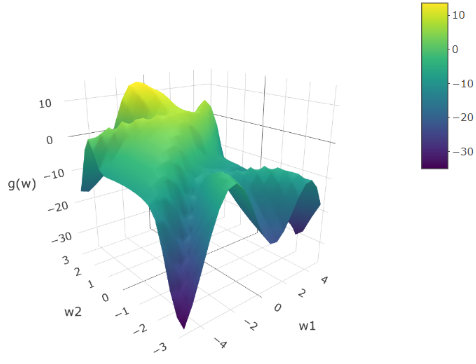
Target Density

- Posterior density priorities:
  i) Predictive risk control, $E[\|\hat{f} - f\|^2]$
  ii) Computational feasibility (i.e. rapid MCMC sampling)
- Train network in a Greedy fashion, add in one neuron at a time
- Previous fit $f_k(x)$ using k neurons, add in new neuron w_{k+1}
- Prior density $p_0(w)$ uniform over ℓ_1 ball, $\|w\|_1 \leq 1$
- For some $\alpha \in [0, 1]$, residuals $r_i = y_i - (1 - \alpha)f_k(x_i)$
- For some gain $\beta > 0$,

$$p_{k+1}(w) \propto e^{\beta \sum_{i=1}^{n} r_i \psi(x_i \cdot w)} p_0(w)$$
$$f_{k+1}(x) = (1 - \alpha)f_k(x) + \beta E_{p_{k+1}}[\psi(x \cdot w)]$$

- **Assume**:
  1) Bounded data entries $|x_{i,j}| \leq 1$ for all i, j
  2) Activation function ψ has bounded second derivative, $|\psi''(u)| \leq c$, example tanh or squared ReLU.

Difficulties Sampling and Multi-Modal Posterior



- Posterior log likelihood:

  $$g(w) = \sum_{i=1}^{n} r_i \, \psi(x_i \cdot w)$$

  $$p(w) \propto e^{\beta g(w)}$$

- (Jones, Ba. 93) greedy pursuit, maximize $g(w)$ to find best next neuron

- However, $g(w)$ is multi-modal and not concave

- $\nabla^2 g(w) = \sum_{i=1}^{n} r_i \, \psi''(x_i \cdot w) x_i x_i^T$ is sum of rank 1 matrices with $\pm$ scaling, not negative definite (i.e. not concave)

Auxiliary Random Variable and Joint Density

- Auxiliary r.v.'s $\xi_i \sim \text{Normal}(\sqrt{\beta |r_i| c}\, x_i \cdot w\ , 1),\ i = 1, \ldots, n$
- Joint density $p(w, \xi) = p(w)p(\xi | w)$
- Pair $(w, \xi) \sim p(w, \xi)$ has correct w marginal $w \sim p(w)$
- By Bayes rule, also have $p(w, \xi) = p(\xi)p(w|\xi)$
- $p(\xi)$: marginal of auxiliary r.v., convolution with normal
- $p(w|\xi)$: reverse conditional, has addition negative definite terms in log likelihood Hessian (will make log concave)
- Goal: first sample a $\xi \sim p(\xi)$ and then sample a $w \sim p(w|\xi)$. If both densities are log concave, MCMC methods will be rapidly mixing

Log Concavity of Reverse Conditional Density

$$
\begin{aligned}
p(w|\xi) &\propto p(w)p(\xi|w) \\
&\propto \exp\left(\beta \sum_{i=1}^{n} r_i \psi(x_i \cdot w) - \frac{1}{2}(\xi_i - \sqrt{\beta |r_i| c}\, x_i \cdot w)^2\right) p_0(w) \\
&\propto \exp\left(\beta \sum_{i=1}^{n} r_i \psi(x_i \cdot w) - \beta |r_i| c \frac{1}{2}(x_i \cdot w)^2 + \sqrt{\beta |r_i| c}\, \xi_i x_i \cdot w\right) p_0(w)
\end{aligned}
$$

$$
\nabla^2 \log p(w) = \beta \sum_{i=1}^{n} \left(r_i \psi''(x_i \cdot w)\right) x_i x_i^T
$$

$$
\nabla^2 \log p(w|\xi) = \beta \sum_{i=1}^{n} \left(r_i \psi''(x_i \cdot w) - |r_i| c\right) x_i x_i^T
$$

- Negative definite term introduced to Hessian
- By assumption $r_i \psi''(x_i \cdot w) - |r_i| c < 0$
- Reverse conditional now log-concave
- Log concave density over convex set rapidly sampled by existing MCMC methods (Applegate, Kannan 91, Lovász, Vempala 07)

Marginal Density of Auxiliary RV

- Marginal density $p(\xi)$ is convolution of target $p(w)$ with normal $p(\xi|w)$
$$p(\xi) = \int p(w)p(\xi|w)dw$$
- Denote $g(w) = \beta \sum_{i=1}^{n} r_i \psi(x_i \cdot w) - \beta |r_i| c \frac{1}{2}(x_i \cdot w)^2$ (concave modified target)
$$\log p(\xi) = -\frac{1}{2}\|\xi\|^2 + \log\left(\int p_0(w) e^{g(w)} e^{\sum_{i=1}^{n} \sqrt{\beta |r_i| c}\, \xi_i x_i w} dw\right)$$
- Negative quadratic (concave, neg def hessian)
- Cumulant generating function (convex, pos def hessian)
- Competition for overall log concavity

Score of Auxiliary RV

- Score, define $|R|$ as diagonal matrix of residuals:

$$\nabla \log p(\xi) = -\xi + E[\sqrt{\beta c}|R|^{\frac{1}{2}} Xw|\xi]$$

- MCMC algorithms need access to score (e.g. Langevin Diffusion)
- Score defined by expectation over log concave density $p(w|\xi)$
- Score estimated empirically via MCMC method on reverse conditional $p(w|\xi)$

Log Concavity of Auxiliary RV

- Hessian:

$$\nabla^2 \log p(\xi) = -I + \mathrm{Cov}[\sqrt{\beta c}|R|^{\frac{1}{2}} X w | \xi]$$

- Log concave if for all unit vector a, direction $v = \sqrt{\beta c}|R|^{\frac{1}{2}} X^T a$

$$\mathrm{Var}(v \cdot w | \xi) \leq 1$$

- Upper bound on maximum eigenvalue of $\mathrm{Cov}[w|\xi]$, i.e. max variance in any direction sufficiently small

Covariance Under Prior

- Want $\mathrm{Var}[v \cdot w | \xi]$
- Consider first prior density $\mathrm{Var}_{p_0}[v \cdot w]$
- Prior $w \sim \mathrm{Uniform}\{w \ s.t. \|w\|_1 \leq 1\}$
- $\mathrm{Cov}_{p_0}[w] \preceq \frac{1}{d^2} I$
- If w drawn from prior, $\mathrm{Cov}_{p_0}[\sqrt{\beta c}|R|^{\frac{1}{2}} X w] \preceq \frac{c\|r\|_\infty \beta n}{d} I$
- **Intuition from prior:** large dimension d can control covariance, d of order $c\|r\|_\infty \beta n$.

Two Proof Methods

1. Contraction Conjecture (not proven):

- Conditional covariance LESS than prior,

$$\mathrm{Cov}[w|\xi] \preceq \mathrm{Cov}_{p_0}[w]$$

- Condition for log concavity: $\frac{c\|r\|_\infty \beta n}{d} < 1$
- With $\beta = \frac{1}{\sqrt{n}}$ need dimension

$$(c\|r\|_\infty)\sqrt{n} < d$$

2. Hölder Inequality Lemma:

- Any direction $v = \sqrt{\beta c}|R|^{\frac{1}{2}} X^T a$,

$$\mathrm{Var}(v \cdot w|\xi) < 20\frac{(c\|r\|_\infty \beta n)^2}{d}$$

- Condition for log concavity, $20\frac{(c\|r\|_\infty \beta n)^2}{d} < 1$
- With $\beta = \frac{1}{\sqrt{n}}$ need dimension

$$20(c\|r\|_\infty)^2 n < d$$

Contraction Conjecture

- $p(w|\xi) \propto p_0(w)e^{\beta g_\xi(w)}$, $g_\xi(w)$ is concave in w
- Would seem to reduce variance in any direction
- When prior $p_0(w)$ is over all of $\mathbb{R}^d$, this is true
- One dimensional marginal in any direction $u = v \cdot w$

$$\frac{d^2}{du^2} \log p(u|\xi) < \frac{d^2}{du^2} \log p_0(u)$$

- One dimensional optimal transport map is a contraction
- Less variance in any direction

- Does NOT hold when $p_0(w)$ restricted to convex set (e.g. uniform over ℓ_1 ball)
- Examples where concave function in one direction increases variance in another
- Example,

$$p(w_1, w_2) \propto e^{-\beta w_2^2} 1\{|w_1| + |w_2| \leq 1\}$$

Increased β INCREASES variance in w_1 direction

Hölder Inequality Proof Sketch

- $\mathrm{Var}(v \cdot w|\xi)$ is not more than

$$\int (v \cdot w)^2 e^{\beta \tilde{g}_\xi(w) - \Gamma_\xi(\beta)} p_0(w) dw$$

where $\tilde{g}_\xi(w)$ is $g_\xi(w)$ minus it's mean under $p_0(w)$

- $\Gamma_\xi(w)$ is cumulant generating function of $\tilde{g}_\xi(w)$
- $\Gamma_\xi(w)$ concave, $\Gamma_\xi(0) = 0, \Gamma'_\xi(0) = 0$
- By Hölders inequality variance is not more than

$$(E_{p_0}[(v \cdot w)^{2\ell}])^{\frac{1}{\ell}} \exp\left\{ \frac{\ell}{\ell - 1} \Gamma_\xi\left(\frac{\ell}{\ell - 1}\beta\right) - \Gamma_\xi(\beta) \right\}$$

- Moments of prior analysis, $(E_{p_0}[(v \cdot w)^{2\ell}])^{\frac{1}{\ell}} < c\|r\|_\infty \beta n^{\frac{4\ell}{ed}}$
- CGF analysis, $\frac{\ell}{\ell-1}\Gamma_\xi(\frac{\ell}{\ell-1}\beta) - \Gamma_\xi(\beta) < c\|r\|_\infty \beta n^{\frac{5}{\ell}}$
- Optimize over ℓ to get bound $20\frac{(c\|r\|_\infty \beta n)^2}{d}$

Summary

- Train single hidden layer NN via sequential Greedy Bayes, residuals $r_i = y_i - (1-\alpha) f_k(x_i)$

$$p_{k+1}(w) \propto e^{\beta \sum_{i=1}^{n} r_i \psi(x_i \cdot w)}$$
$$f_{k+1}(x) = (1-\alpha) f_k(x) + \beta E_{p_k}[\psi(x \cdot w)]$$

- Define joint density $p(w, \xi)$ with correct w marginal
- $p(w|\xi)$ log concave and can be sampled via MCMC
- Marginal $p(\xi)$ has score which can be estimated via MCMC sampling over $p(w|\xi)$:

$$\nabla \log p(\xi) = -\xi + E[\sqrt{\beta c}|R|^{\frac{1}{2}} X w | \xi]$$

- $p(\xi)$ is log concave for large dimension d:
  - (Conjectured) Log-concave when $c\|r\|_\infty \beta n < d$
  - (Proven) Log-concave when $20(c\|r\|_\infty \beta n)^2 \leq d$

Future Work: Predictive Risk Control

- Statistical risk or generalization squared error: $E[\|\hat{f} - f\|^2]$
- Use multiple subsets of data $1 \leq n \leq N$
  - Predictive density: $p_n(y|x) = \int p(y|x, w)p(w|x^n, y^n)dw$
  - Predictive mean: $\hat{f}_n(x) = \int f(x, w)p(w|x^n, y^n)dw$
  - Cumulative estimator: $\hat{\hat{f}}(x) = \frac{1}{N}\sum_{n=1}^{N} \hat{f}_n(x)$
- Upper bound with Kullback divergence,

$$E[\|\hat{\hat{f}} - f\|^2] \leq \frac{1}{N} D(P^*_{Y^N,X^N} \| P_{Y^N,X^N})$$

- Index of resolvability (Ba. 87, 98):

$$\begin{aligned}
\frac{1}{N} D(P^*_{Y^N,X^N} \| P_{Y^N,X^N}) &= \frac{1}{N} E[\log \frac{p^*(y^N, x^N)}{\int p(y^N, x^N|w)p_0(w)dw}] \\
&\leq \frac{1}{N} E[\log \frac{p^*(y^N, x^N)}{\int_A p(y^N, x^N|w)p_0(w)dw}] \\
&\leq D_A + \frac{1}{N} \log \frac{1}{P_0(A)}
\end{aligned}$$

- Prior probability control $P_0(A)$, Gaussian not sufficient, need uniform prior
- Best bounds to date: $E[\|\hat{\hat{f}} - f\|^2] \leq C\left(\frac{(\log 2d)}{N}\right)^{\frac{1}{3}}$

THE END

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