SLANG: Fast Structured Covariance Approximations for Bayesian Deep Learning with Natural Gradient

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Introduction

Motivation:

- Uncertainty estimation is essential to make reliable decisions based on the predictions of deep models, but is computationally challenging.
- It is difficult to form even a Gaussian approximation to the posterior for large models.
- Mean-field methods reduce the computational complexity, but yield poor estimates of the uncertainty.

Contributions:

- We propose a new **stochastic, low-rank, approximate natural-gradient (SLANG)** method for Gaussian variational inference.
- Our method estimates a "low-rank plus diagonal" covariance matrix based solely on back-propagated gradients.
- SLANG is faster and more accurate than mean-field methods, and performs comparably to state-of-the-art methods.

Natural Gradient Variational Inference

Given a deep model $p(\mathcal{D}|\boldsymbol{\theta})$ with weights $\boldsymbol{\theta}$, **Gaussian Variational Inference** computes a Gaussian approximation $q(\boldsymbol{\theta}) := \mathcal{N}(\boldsymbol{\theta}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$ to the posterior by maximizing the ELBO:

$$\mathcal{L}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \mathbb{E}_q \left[\log p(\mathcal{D}|\boldsymbol{\theta}) + \log \mathcal{N}(\boldsymbol{\theta} \mid 0, \mathbf{I}/\lambda) - \log q(\boldsymbol{\theta})\right],$$

Gradient-based methods optimize the ELBO using the stochastic gradient updates (t is the iteration, γ_t is the learning rate)

$$\boldsymbol{\mu}_{t+1} = \boldsymbol{\mu}_t - \gamma_t \hat{\nabla}_{\mu}\mathcal{L}_t, \qquad \boldsymbol{\Sigma}_{t+1} = \boldsymbol{\Sigma}_t - \gamma_t \hat{\nabla}_{\Sigma}\mathcal{L}_t.$$

Problem: Gradient descent implicity uses Euclidean geometry.

↓

Natural Gradient methods do steepest descent in the space of realizable variational distributions $q(\theta)$ by optimizing on the Riemannian manifold. This gives the update

$$\boldsymbol{\mu}_{t+1} = \boldsymbol{\mu}_t - \beta_t \boldsymbol{\Sigma}_{t+1} \hat{\nabla}_{\mu}\mathcal{L}_t \qquad \boldsymbol{\Sigma}_{t+1}^{-1} = (1-\beta_t)\boldsymbol{\Sigma}_t^{-1} + \beta_t \hat{\nabla}_{\Sigma}\mathcal{L}_t.$$

Problem: This update requires computing the Hessian.

↓

Variational Online Gauss-Newton approximates the Hessian with the empirical Fisher Information matrix $\hat{\mathbf{G}}(\theta_t)$. This gives

$$\boldsymbol{\mu}_{t+1} = \boldsymbol{\mu}_t - \beta_t \boldsymbol{\Sigma}_{t+1}\left[\hat{g}(\theta_t) + \lambda \boldsymbol{\mu}_t\right]$$
$$\boldsymbol{\Sigma}_{t+1}^{-1} = (1-\beta_t)\boldsymbol{\Sigma}_t^{-1} + \beta_t \left[\hat{\mathbf{G}}(\theta_t) + \lambda \mathbf{I}\right],$$

where $\hat{g}(\theta_t)$ is the gradient and

$$\hat{\mathbf{G}}(\theta_t) = \frac{1}{M}\sum_{i=1}^{M} g_i(\theta_t) g_i(\theta_t)^\top$$

is the empirical Fisher Information matrix for $p(\mathcal{D} \mid \theta_t)$ computed with a minibatch of size M.

Problem: Computing and storing $\boldsymbol{\Sigma}_t$ is $O(D^2)$ for dense covariances.

SLANG

We approximate the covariance with a "low-rank plus diagonal" matrix

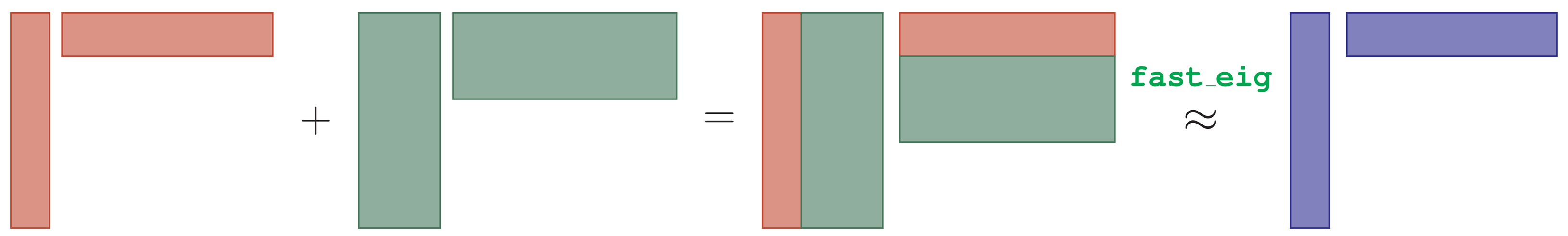
$$\boldsymbol{\Sigma}_t^{-1} \approx \hat{\boldsymbol{\Sigma}}_t^{-1} := \mathbf{U}_t\mathbf{U}_t^\top + \mathbf{D}_t,$$

where $\mathbf{U}_t$ is a $D \times L$ matrix and $\mathbf{D}_t$ is diagonal. The cost of storing and inverting this matrix is linear in D which is reasonable when $L \ll D$.
The approximate natural gradient update for $\hat{\boldsymbol{\Sigma}}_t^{-1}$ is

$$\hat{\boldsymbol{\Sigma}}_{t+1}^{-1} := \mathbf{U}_{t+1}\mathbf{U}_{t+1}^\top + \mathbf{D}_{t+1} \approx (1-\beta_t)\hat{\boldsymbol{\Sigma}}_t^{-1} + \beta_t\left[\hat{\mathbf{G}}(\theta_t) + \lambda\mathbf{I}\right]$$

This update may increase the rank of $\mathbf{U}_{t+1}$, so we project the matrix onto a L-dimensional subspace using an eigenvalue decomposition:

$$(1-\beta_t)\hat{\boldsymbol{\Sigma}}_t^{-1} + \beta_t\left[\hat{\mathbf{G}}(\theta_t) + \lambda\mathbf{I}\right] = \underbrace{(1-\beta_t)\mathbf{U}_t\mathbf{U}_t^\top + \beta_t\hat{\mathbf{G}}(\theta_t)}_{\text{Rank at most } L+M} + \underbrace{(1-\beta_t)\mathbf{D}_t + \beta_t\lambda\mathbf{I}}_{\text{Diagonal component}},$$
$$\approx \underbrace{\mathbf{Q}_{1:L}\boldsymbol{\Lambda}_{1:L}\mathbf{Q}_{1:L}^\top}_{\text{Rank } L \text{ eigendecomposition}} + \underbrace{(1-\beta_t)\mathbf{D}_t + \beta_t\lambda\mathbf{I}}_{\text{Diagonal component}}.$$



$(1-\beta)\mathbf{U}_t\mathbf{U}_t^\top$ $\beta\mathbf{G}(\theta_t)$ $\mathbf{U}_{t+1}\mathbf{U}_{t+1}^\top$

The diagonal information lost in this projection is equal to

$$\Delta_D = \operatorname{diag}\left[(1-\beta)\mathbf{U}_t\mathbf{U}_t^\top + \beta_t\hat{\mathbf{G}}(\theta_t) - \mathbf{U}_{t+1}\mathbf{U}_{t+1}^\top\right].$$

We add this to $\mathbf{D}_t$ as a diagonal correction. The final SLANG update is

$$\textbf{SLANG:} \quad \mathbf{U}_{t+1} = \mathbf{Q}_{1:L}\boldsymbol{\Lambda}_{1:L}^{1/2}$$
$$\mathbf{D}_{t+1} = (1-\beta)\mathbf{D}_t + \beta_t\lambda\mathbf{I} + \Delta_D.$$
$$\boldsymbol{\mu}_{t+1} = \boldsymbol{\mu}_t - \alpha_t\left[\mathbf{U}_{t+1}\mathbf{U}_{t+1}^\top + \mathbf{D}_{t+1}\right]^{-1}\left[\hat{\mathbf{g}}(\theta_t) + \lambda\boldsymbol{\mu}_t\right].$$

The Algorithm

Pseudo-code for SLANG is shown in Algorithm 1. α, β are learning rates, D is denoted with a vector $\mathbf{d}$ and $\mathbf{u}_j$ and $\mathbf{v}_j$ are the columns of $\mathbf{U}$ and $\mathbf{V}$, respectively.

Algorithm 1: `SLANG`

Require: Data $\mathcal{D}$, hyperparameters $M, L, \lambda, \alpha, \beta$
Initialize $\boldsymbol{\mu}, \mathbf{U}, \mathbf{d}$
$\delta \leftarrow (1-\beta)$
while not converged **do**
  $\boldsymbol{\theta} \leftarrow$ `fast_sample`$(\boldsymbol{\mu}, \mathbf{U}, \mathbf{d})$
  $\mathcal{M} \leftarrow$ sample a minibatch
  $[\mathbf{g}_1, .., \mathbf{g}_M] \leftarrow$ `backprop`$(\mathcal{D}_{\mathcal{M}}, \boldsymbol{\theta})$
  $\mathbf{V} \leftarrow$ `fast_eig`$(\delta\mathbf{u}_1, .., \delta\mathbf{u}_L, \beta\mathbf{g}_1, .., \beta\mathbf{g}_M, L)$
  $\Delta_d \leftarrow \sum_{i=1}^{L}\delta\mathbf{u}_i^2 + \sum_{i=1}^{M}\beta\mathbf{g}_i^2 - \sum_{i=1}^{L}\mathbf{v}_i^2$
  $\mathbf{U} \leftarrow \mathbf{V}$
  $\mathbf{d} \leftarrow \delta\mathbf{d} + \Delta_d + \lambda\mathbf{1}$
  $\hat{\mathbf{g}} \leftarrow \sum_i \mathbf{g}_i + \lambda\boldsymbol{\mu}$
  $\Delta_\mu \leftarrow$ `fast_inverse`$(\hat{\mathbf{g}}, \mathbf{U}, \mathbf{d})$
  $\boldsymbol{\mu} \leftarrow \boldsymbol{\mu} - \alpha\Delta_\mu$
end while
return $\boldsymbol{\mu}$, $\mathbf{U}$, $\mathbf{d}$

Algorithm 2: `fast_inverse`$(\mathbf{g}, \mathbf{U}, \mathbf{d})$

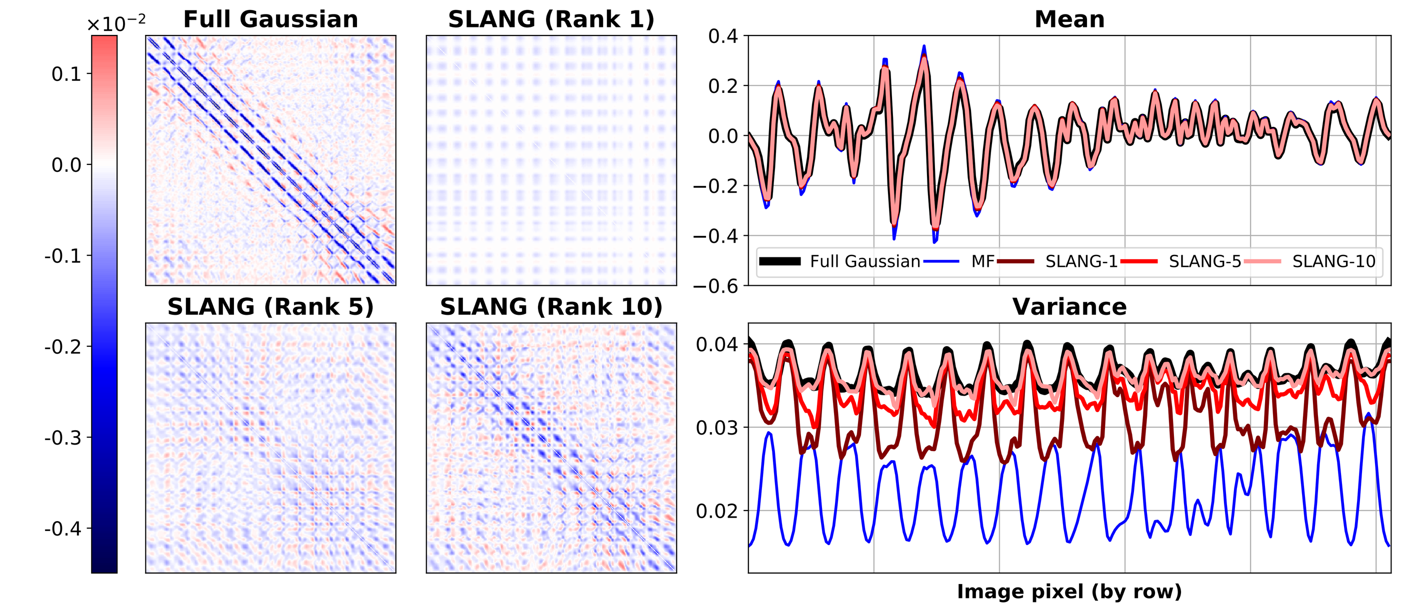
$\mathbf{A} \leftarrow (\mathbf{I}_L + \mathbf{U}^\top\mathbf{d}^{-1}\mathbf{U})^{-1}$
$\mathbf{y} \leftarrow \mathbf{d}^{-1}\mathbf{g} - \mathbf{d}^{-1}\mathbf{U}\mathbf{A}\mathbf{U}^\top\mathbf{d}^{-1}\mathbf{g}$
return $\mathbf{y}$

Algorithm 3: `fast_sample`$(\boldsymbol{\mu}, \mathbf{U}, \mathbf{d})$

$\epsilon \sim \mathcal{N}(0, \mathbf{I}_D)$
$\mathbf{V} \leftarrow \mathbf{d}^{-1/2} \odot \mathbf{U}$
$\mathbf{A} \leftarrow \text{Cholesky}(\mathbf{V}^\top\mathbf{V})$
$\mathbf{B} \leftarrow \text{Cholesky}(\mathbf{I}_L + \mathbf{V}^\top\mathbf{V})$
$\mathbf{C} \leftarrow \mathbf{A}^{-\top}(\mathbf{B} - \mathbf{I}_L)\mathbf{A}^{-1}$
$\mathbf{K} \leftarrow (\mathbf{C} + \mathbf{V}^\top\mathbf{V})^{-1}$
$\mathbf{y} \leftarrow \mathbf{d}^{-1/2}\epsilon - \mathbf{V}\mathbf{K}\mathbf{V}^\top\epsilon$
return $\boldsymbol{\mu} + \mathbf{y}$

Results

Covariance Structure for Logistic Regression on USPS



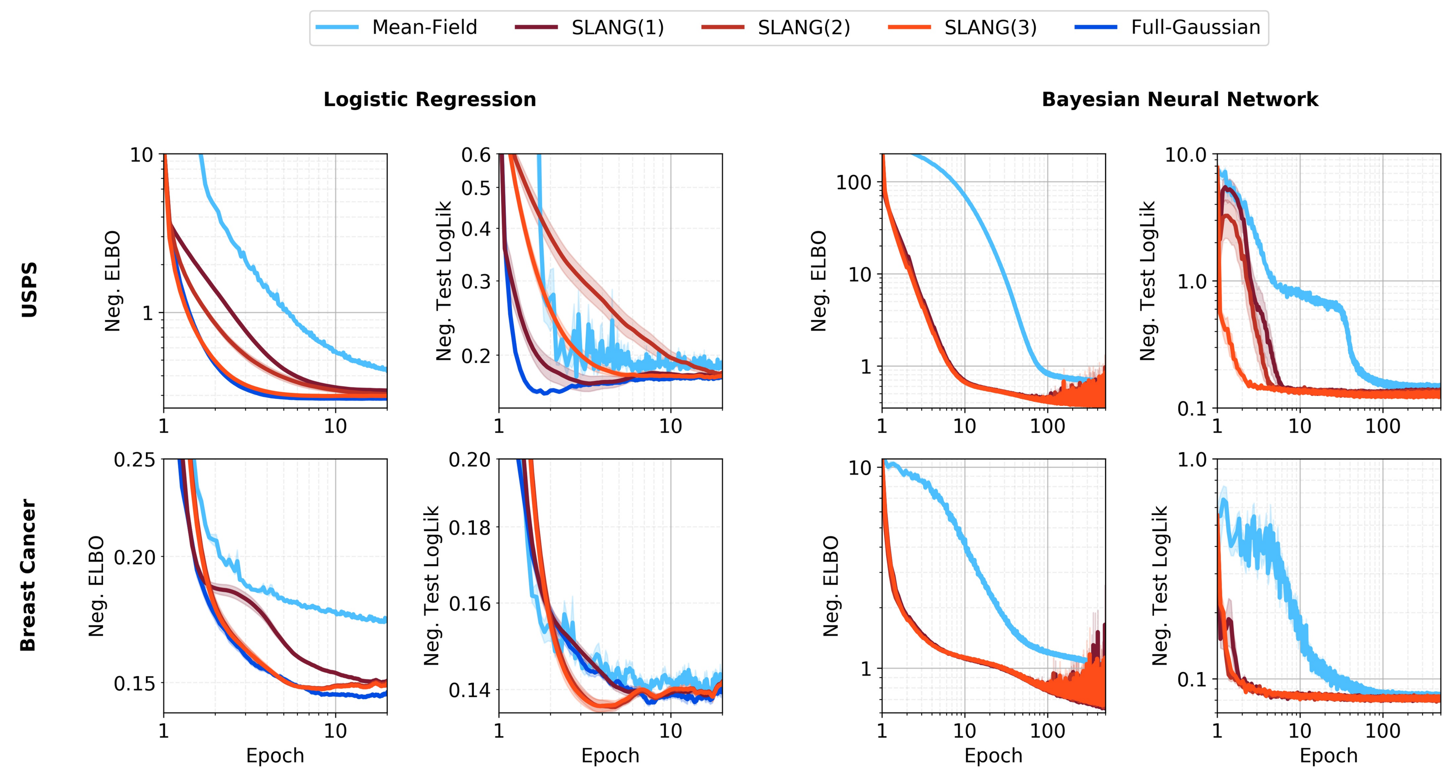
- SLANG doesn't underestimate variance like mean-field methods.

Logistic Regression Results

Dataset	Metrics	Mean-Field Methods EF	Hess.	Exact	SLANG L = 1	L = 5	L = 10	Full Gaussian EF	Hess.	Exact
Australian	NLL	0.348	0.347	0.341	0.342	0.339	**0.338**	0.340	0.339	0.338
	KL ($\times 10^4$)	2.240	2.030	0.195	0.033	0.008	**0.002**	0.000	0.000	0.000
a1a	NLL	0.339	0.339	0.339	0.339	0.339	**0.339**	0.339	0.339	0.339
	KL ($\times 10^2$)	2.590	2.208	1.295	0.305	0.173	**0.118**	0.014	0.000	0.000
USPS 3vs5	NLL	0.139	0.139	0.138	0.132	0.132	**0.131**	0.131	0.130	0.130
	KL ($\times 10^1$)	7.684	7.188	7.083	1.492	0.755	**0.448**	0.180	0.001	0.000

- SLANG performs similarly to full-Gaussian methods at test time.

Convergence Experiments



- SLANG converges faster than mean-field methods for logistic regression and BNNs.

Bayesian Neural Networks Results:

Dataset	Test RMSE BBB	Dropout	SLANG	Test log-likelihood BBB	Dropout	SLANG
Boston	3.43 ± 0.20	**2.97 ± 0.19**	3.21 ± 0.19	-2.66 ± 0.06	**-2.46 ± 0.06**	-2.58 ± 0.05
Concrete	6.16 ± 0.13	**5.23 ± 0.12**	5.58 ± 0.19	-3.25 ± 0.02	**-3.04 ± 0.02**	-3.13 ± 0.03
Energy	0.97 ± 0.09	1.66 ± 0.04	**0.64 ± 0.03**	-1.45 ± 0.10	-1.99 ± 0.02	**-1.12 ± 0.01**
Kin8nm	0.08 ± 0.00	0.10 ± 0.00	**0.08 ± 0.00**	**1.07 ± 0.00**	0.95 ± 0.01	1.06 ± 0.00
Naval	0.00 ± 0.00	0.01 ± 0.00	**0.00 ± 0.00**	4.61 ± 0.01	3.80 ± 0.01	**4.76 ± 0.00**
Power	4.21 ± 0.03	**4.02 ± 0.04**	4.16 ± 0.04	-2.86 ± 0.01	**-2.80 ± 0.01**	-2.84 ± 0.01

- Performance on BNNs is comparable to Bayesian Dropout and Bayes-by-Backprop.