

A Full Method Description

ADVI Baseline

Uses a full-rank Gaussian initialized to standard normal and optimizes with closed-form entropy gradient from Equation (2); uses ADVI step-scheme for updates (see Appendix D for more details). Importance-weighted sampling is not used; importance-weighted training is not used (optimized standard ELBO).

Method (0)

Uses a full-rank Gaussian initialized to standard normal and optimizes with closed-form entropy gradient from Equation (2); uses our comprehensive step-size search for updates (see Section 3.2 for more details). Importance-weighted sampling is not used; importance-weighted training is not used.

Method (1)

Uses a full-rank Gaussian initialized to standard normal and optimizes with the STL from Equation (3); uses our comprehensive step-size search for updates. Importance-weighted sampling is not used; importance-weighted training is not used.

Method (2)

Uses a full-rank Gaussian and initializes with LI method from Section 3.4; optimizes with the STL from Equation (3) and uses our comprehensive step-size search for updates. Importance-weighted sampling is not used; importance-weighted training is not used.

Method (3a)

Uses a full-rank Gaussian initialized to standard normal and optimizes with the STL gradient from Equation (3); uses our comprehensive step-size search for updates. Importance-weighted sampling is used with $M = 10$; importance-weighted training is not used.

Method (3b)

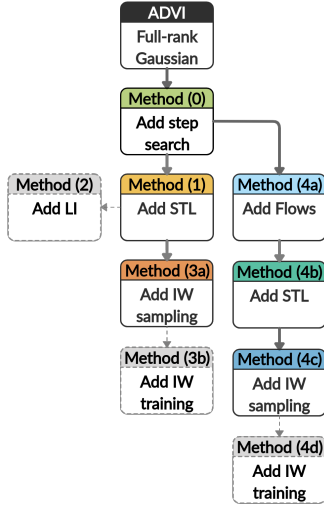
Uses a full-rank Gaussian initialized to standard normal and uses importance-weighted training with $M = 10$; optimizes with the DReG from Equation (6) and uses our comprehensive step-size search for updates. Importance-weighted training is used with $M = 10$ (optimizes IW-ELBO with $M = 10$).

Method (4a)

Uses a real-NVP normalizing flow (see Appendix E for architectural and initialization details) as q_ϕ ; optimizes with the “full” gradient from Equation (3) and uses our comprehensive step-size search for updates. Importance-weighted sampling is not used; importance-weighted training is not used.

Method (4b)

Uses a real-NVP normalizing flow and optimizes with the STL gradient from Equation (3); uses our comprehensive step-size search for updates. Importance-weighted sampling is not used; importance-weighted training is not used.



Method (4c)

Uses a real-NVP normalizing flow and optimizes with the STL gradient from Equation (3); uses our comprehensive step-size search for updates. Importance-weighted sampling is used with $M = 10$; importance-weighted training is not used.

Method (4d)

Uses a real-NVP normalizing flow and uses importance-weighted training with $M = 10$; optimizes with the DReG gradient from Equation (6) and uses our comprehensive step-size search for updates. Importance-weighted training is used with $M = 10$.

B Extended results

B.1 Diagonal vs Full-rank Gaussian VI

In this section, we compare the performance of Gaussian VI with full-rank covariance against diagonal covariance. While it is well known that full-rank covariance Gaussian distribution are more expressive, a clear experimental evidence for this is notably missing from the literature—we supplement this by experimenting with three methods from our path-study: Method (0), Method (1), and Method (3a). In Figure 11, it is easy to observe that using full-rank Gaussian improves performance by 1 nats or more on at least half of the models across the methods. When using Importance Weighted sampling—Method (3a)—full-rank covariance Gaussians almost always improves the performance.

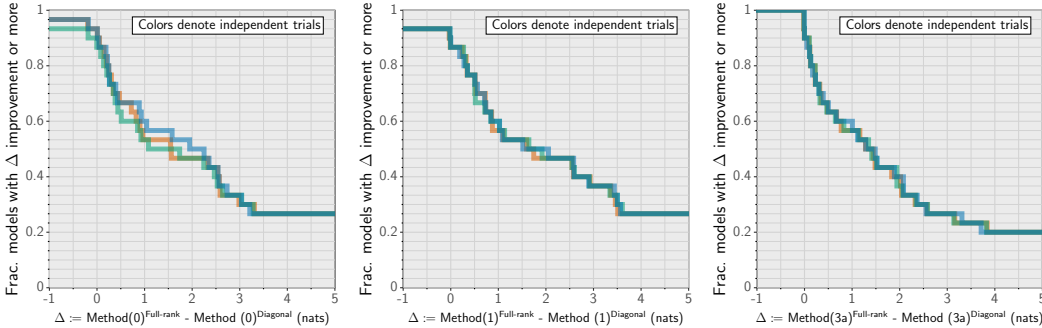


Figure 11: Full-rank vs. Diagonal: (a) Method (0): closed-form entropy w/ step search, (b) Method (1): we replace closed-form entropy with STL gradient, and (c) Method (3a): we add Importance Weighted Sampling to STL gradient. In all the methods, using full-rank Gaussian improves the performance by at least 1 nats on more than half of the models.

B.2 Different gradient for Gaussian VI

There are three choices of gradients for the Gaussian family. First, as Gaussians have a closed-form entropy, we can use the gradient from Equation (2); this is the gradient that ADVI uses. Second, we can alternatively use the middle gradient from Equation (3). Third, we can drop the score-function term and use the STL estimator (third term in Equation (3)). In Figure 12, the first panel compares the performance of using STL against the ADVI implementation (ADVI step-scheme and gradient). In the second panel, we compare the performance with the closed-form estimator optimized using our comprehensive step-search. Finally, we compare against the middle gradient in Equation (3). In all the alternatives, STL rarely hurts and adds significant value to several models.

B.3 IW-training with DReG

We compare IW-training with and without DReG estimator on different possibilities and find that it consistently improved the performance. In Figure 13, we first compare the performance with the standard IW-ELBO gradient for Gaussian families. In the second comparison, we add Laplace Initialization to both methods, IW-ELBO gradient and DReG gradient. In the final comparison, we

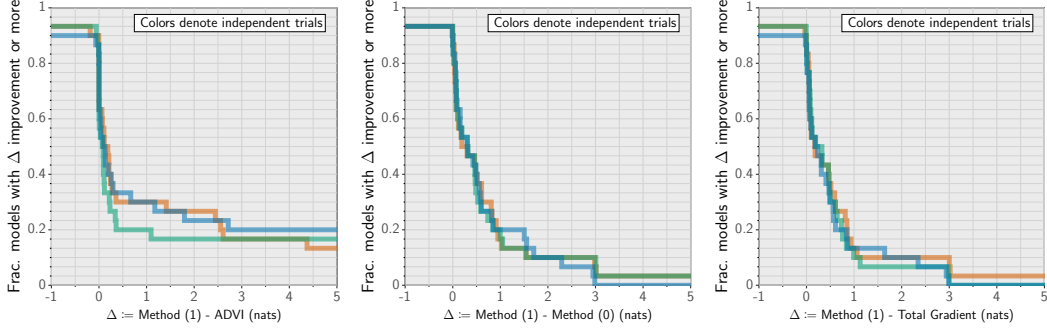


Figure 12: (a) STL against ADVI; STL improves the performance by 1 nat or more on almost 30% of the models. (b) Next, we replace the ADVI step-size scheme with our comprehensive step search. STL improves the performance on 20% of the models by 1 nat or more. (c) We also compare against the middle gradient from Equation (3) and find that STL provides an improvement of 1 nat or more on almost 10% of the models. In all the alternatives, STL rarely hurts.

compare DReG with regular IW-ELBO gradient for normalizing flows. Across all comparisons, DReG improves the performance and rarely hurts.

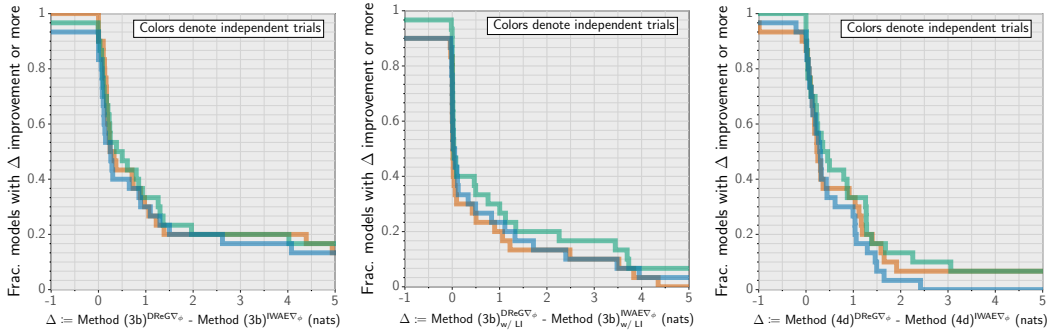


Figure 13: (a) DReG improves the performance significantly by 1 nat on almost 30% of the models for Gaussians when initialized with standard normal (b) On adding LI to the previous model, DReG adds 1 nat to around 20% of the models (c) Adding DReG to IW-training of flows also helps. We observe significant improvement of 1 nat or more for almost 30% of the models

B.4 Path Study - full results

We conduct a path-study to accumulate all the useful combinations of our analysis. Figure 15 presents the study for three independent trials. The high variation is due to the ADVI; on 10 models out of 30, ADVI diverges in at-least one trial for our implementation. If an optimization diverges, we set the improvement as zero, that is, we count the model in favor of the baseline (see Table 2 for values).

B.5 Ablation Study - full results

We conduct an ablation-study to analyze each component of the best performing method. Figure 16 presents the study for three independent trials.

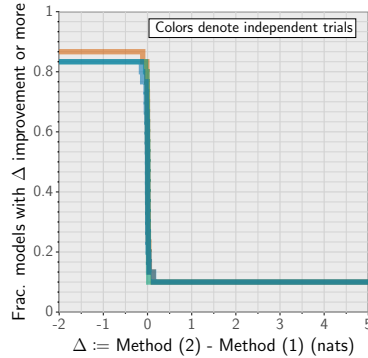


Figure 14: Adding LI to Gaussian VI is neither consistently helpful nor consistently harmful.

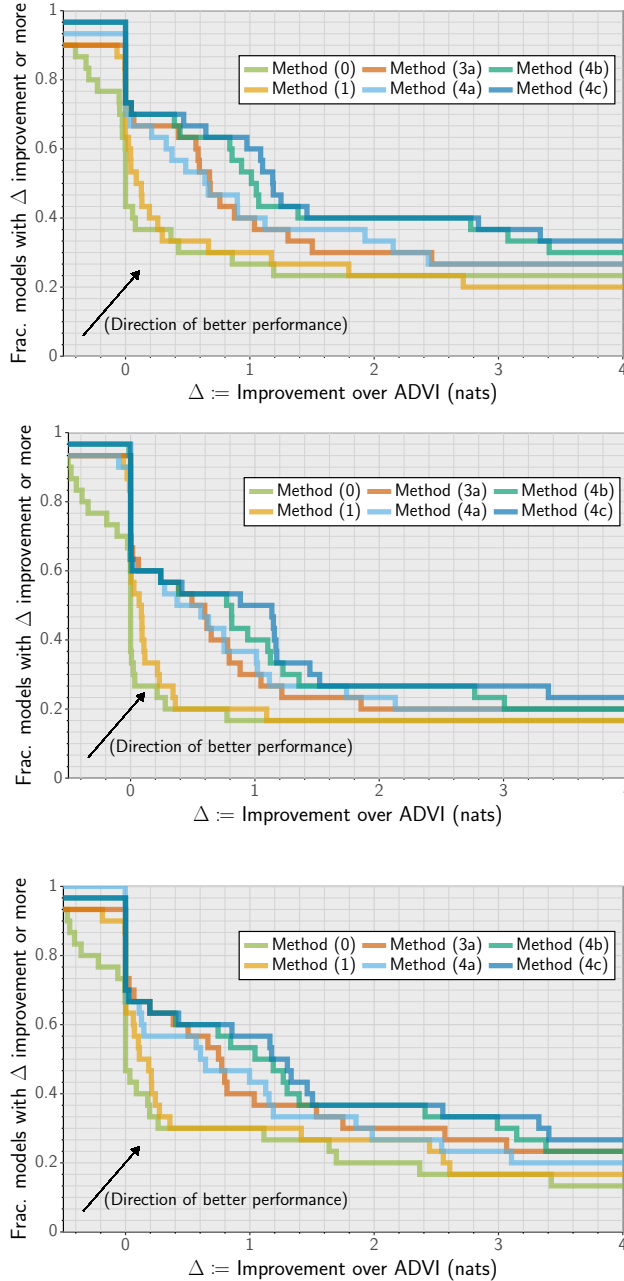


Figure 15: Across the trials: Method (1) that uses STL gradient improves over ADVI by 1 nat or more for at least 20% of the models. Method (3a) adds the IW-sampling to (1) and improves by a nat or more on at least 30% of the models. Method (4a) uses flow with the naive gradient estimator and achieves performance similar to (3a). Method (4b) adds the STL gradient to (4a) and improves on at least 40% of the models by 1 nat or more. Method (4c) adds IW-sampling to (4b) and improves by 1 nat on a minimum of 50% of the models. All our methods use comprehensive step-search and use $M = 10$ wherever IW-sampling is applied.

B.6 Laplace Initialization

Figure 14 compares the results of using Laplace initialization (LI) against not using it (we omitted this comparison from the main text for brevity). While there is a significant improvement on a minority of models, similar fraction observe a significant decay.

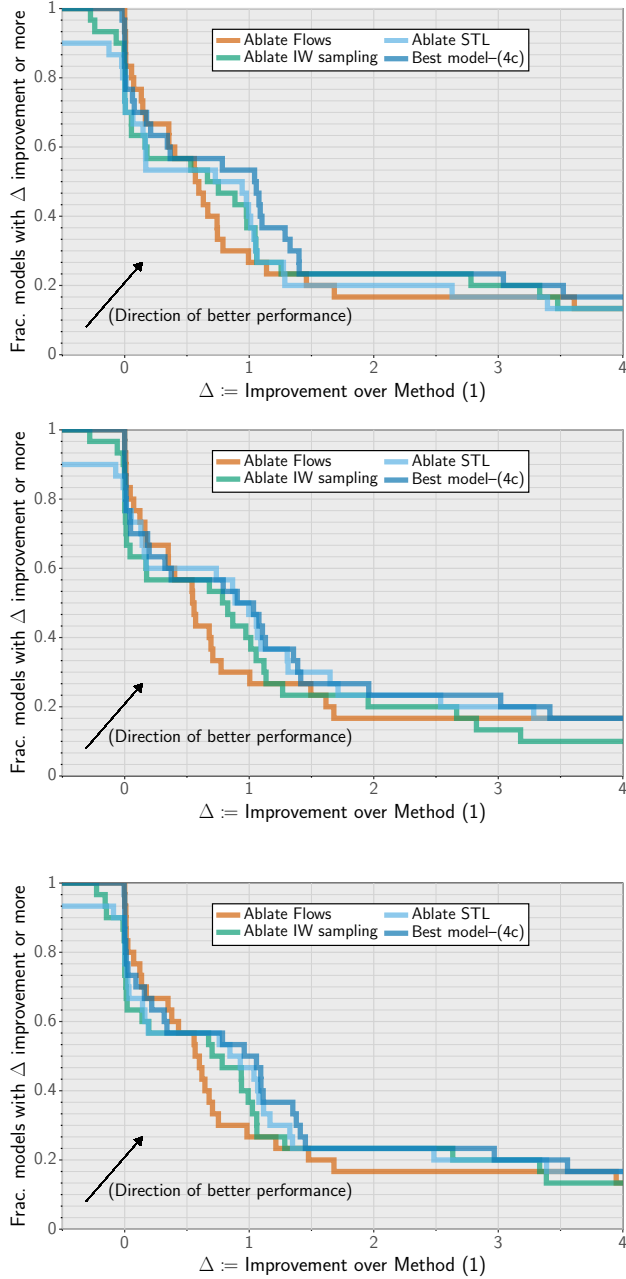


Figure 16: Across the trials: ablating STL observes the least decay in performance while ablating flows causes the most decrease. The effect of ablating IW-sampling lies somewhere in the middle of these two. All approaches are trained with comprehensive step-search and use $M=10$ wherever importance weighted sampling is used.

C Interfacing using auto-diff packages

To interface with Stan models, we must define a new “primitive” function in Autograd that corresponds to $\log p(x, z)$ as a function of z . In addition, this also requires computing $\log p(x, z)$ itself as well as the gradient-vector product $a^\top \nabla_z \log p(z, x)$ for any vector a . This is easily done since PyStan interface allows access to $\log p(z, x)$ and the gradient $\nabla_z \log p(z, x)$ for any model defined in Stan. This approach has the disadvantage that high-order gradients are not possible. Similar strategies could be used with other automatic differentiation packages.

D ADVI

Step-size scheme ADVI uses a novel step-size sequence inspired by adaptive step-size gradient schemes [12, 29, 17]. The update at iteration i is

$$\phi^{(i+1)} = \phi^{(i)} - \rho^{(i)} \odot g^{(i)}, \quad (9)$$

where $g^{(i)}$ is the stochastic gradient in the i -th iteration, $\rho^{(i)}$ is a vector of step-sizes (one per coordinate of ϕ) and \odot denotes elementwise multiplication. To determine the stepsizes, a vector $s^{(i)}$ is initialized to $s^{(1)} = (g^{(1)})^2$ and maintained recursively as

$$s^{(i)} = \alpha(g^{(i)})^2 + (1 - \alpha)s^{(i-1)}, \quad (10)$$

Then, the stepsizes are chosen as

$$\rho^{(i)} = \frac{\eta}{i^{1/2+\epsilon} \times (\tau + \sqrt{s^{(i)}})}, \quad (11)$$

where the square root and division are element-wise. Here $\eta > 0$ is the scale of the step-size, $i^{1/2+\epsilon}$ decays the step over time, and the $s^{(i)}$ adapts the curvature of the ELBO. $\tau = 1$ and $\epsilon = 10^{-16}$ are stabilizing constants.

Implementation details ADVI step-scheme search for η from Equation (11) over the range $\{0.01, 0.1, 1, 10, 100\}$ to best adapt to the size of the problem. We use 200 optimization iterations for each of these choices and then use a fresh batch of 500 samples for each step in the range to calculate final ELBO values. The step with highest final ELBO is selected as the adapted step-size; with the adapted η we optimize for 30,000 iterations where, at each iteration we use 100 total log p evaluation (same as our other experiments).

We also implement the relative-tolerance convergence criterion implemented in PyStan to detect early convergence (we use a tolerance of 0.001). Also, following the original work, we use the closed form of entropy of q_ϕ for the ADVI training objective. We make an honest attempt to the best of our abilities to re-implement the ADVI and in our preliminary experiments found that the performance matched the PyStan version for the same hyper-parameter settings. We found that the performance of ADVI was highly variable; out of the three independent trials, 9 models diverged in at least one trial. Replacing ADVI step-scheme with our comprehensive step-search saw no divergence for the closed-form entropy case that uses Adam optimizer.

E Implementation details for real-NVP

Architectural details: We use a real-NVP flow with 10 coupling layers for all our experiments. We define each coupling layer to be comprised of two transitions, where a single transition corresponds to affine transformation of one part of the latent variables. For example, if the input variable for the k^{th} layer is $z^{(k)}$, then first transition is defined as

$$\begin{aligned} z_{1:d} &= z_{1:d}^{(k)} \\ z_{d+1:D} &= z_{d+1:D}^{(k)} \odot \exp(s_k^a(z_{1:d}^{(k)})) + t_k^a(z_{1:d}^{(k)}). \end{aligned} \quad (12)$$

where, super-script a denotes first transition and sub-script k denotes the k^{th} layer. For the next transition, the $z_{d+1:D}$ part is kept unchanged and $z_{1:d}$ is affine transformed in a similar fashion to obtain the layer output $z^{(k+1)}$ (this time using $s_k^b(z_{d+1:D}^{(k)})$ and $t_k^b(z_{d+1:D}^{(k)})$). This is also referred to as the alternating first half binary mask. Both, scale(s) and translation(t) functions are parameterized by the same fully connected neural network(FNN). More specifically, for first transition in above example, a single FNN takes $z_{1:d}^{(k)}$ as input and outputs both $s_k^a(z_{1:d}^{(k)})$ and $t_k^a(z_{1:d}^{(k)})$. Thus, the skeleton of the FNN, in terms of the size of the layers, is as $[d, H, H, 2(D-d)]$ where, H denotes the size of the two hidden layers ($H=32$ for all our experiments).

The hidden layers of FNN use a leaky rectified linear unit with slope = 0.01, while the output layer uses a hyperbolic tangent for s and remains linear for t .

Parameter Initialization: We initialize the parameters of the neural networks from normal distribution $\mathcal{N}(0, 0.001^2)$. We deliberately make this choice as it corresponds to an approximate standard normal initialization for the overall normalizing flow density. To see this, first note that the output from the initialized neural networks will approximately be 0 vectors. Now, consider the affine transformation of real-NVP: at each iteration, we scale by the exponent of s and offset by t . Thus, the overall effect is an identity transform. As the base-distribution is fixed to a standard normal, this gives as an approximate standard normal initialization.

Number of Parameters: For each transition, assuming $d = D/2$, the parameters of the FNN can be calculated as $\frac{1}{2}DH + H^2 + HD + D + 2H$ where D is the number latent dimensions in the model, and H is the size of the two hidden layers. The first three components in the calculation corresponds to weight matrix, and the latter two take into account the bias parameters. With T coupling layers, each comprising of 2 transitions, the overall parameter size is given by $2T(\frac{3}{2}DH + H^2 + D + 2H)$. We use $T=10$ and $H=32$, while D depends on the problem.

Scaling to higher dimension models: Real NVP based architectures scale better to higher dimensional problems as compared to Gaussians. The parameters in Gaussian scale as $\mathcal{O}(D^2)$ while they scale linearly $\mathcal{O}(D)$ for real-NVP, if we fix other parameters(T and H). However, for lower dimensional problem the number of parameters for real-NVP is more.

F Selection of Best model

We choose the model that achieves best average-objective, averaged over the entire optimization trace. This is different from, perhaps a more natural, final value based selection rule where one evaluates on a smaller batch of fresh samples; smaller compared to number of samples used for final metric evaluation. We found average objective to be more reliable indicator of the performance in practice. In our preliminary experiments, models selected from the maximum average-objective out-performed the ones selected based on the maximum final value; the comparison was based on the final metric value evaluated using a fresh batch of 10,000 samples.

G Full list of models

We present the complete list of models used in our analysis [Table 1](#). The descriptions in the table have been manually extracted, see Stan-example model repository [\[35\]](#) for more details.

H Complete Table of results

Table 1: This table presents attributes of all the models from the Stan model library [35, 36] that have been used in this analysis. The attribute are $|z| = \#$ of latent dimensions, $n = \#$ of data points, and $r = \frac{\# \text{ of latent dimensions}}{\# \text{ of data points}}$

Id	Model name	$ z $	n	r	Model Description
1	lsat	1006	818	1.2298	One-parameter Rasch model for LSAT student response
2	Mh	388	385	1.0078	Heterogeneity model for closed population size estimation from capture-recapture data with individual effects
3	test_simplex	3	10	0.3000	Simplex estimator
4	endo3	184	626	0.2939	Conditional inference model for case-control study on endometrial cancer
5	gp_predict	265	989	0.2679	Model for predicting out-of-sample observations by fitting hyperparams of a latent variable Gaussian process with exponentiated quadratic kernel and Gaussian likelihood
6	Mth	394	1935	0.2036	Combined model for for closed population size estimation with both, time and individual effects
7	oxford	244	1226	0.1990	A mixture model for the log odds ratio to analyze Oxford childhood cancer data
8	cjs_mnl	22	132	0.1667	CJS model for capture-recapture problem with multinomial likelihood
9	hepatitis	218	1596	0.1366	Normal hierarchical model with measurement error in Hb titre in children post Hepatitis vaccination
10	normal_multi	100	826	0.1211	Basic Multi-variate estimators for normal and student-t distributions
11	hiv_chr	173	1476	0.1172	Multi-level linear model with varying slope and intercept for Zinc diet experiment on HIV positive children
12	electric_1c_chr	116	1248	0.0929	Multi-level linear model with varying intercept and slope for the effect of exposure to television show, The Electric Company
13	electric_1a_chr	112	1248	0.0897	Multi-level linear model with group level factors for the effect of exposure to television show, The Electric Company
14	electric_chr	100	1248	0.0801	Multi-level linear model with varying intercept for the effect of exposure to television show, The Electric Company
15	radon_vary_si_chr	175	4595	0.0381	Multi-level linear model with group level predictors to estimate radon levels.
16	lda	33	1157	0.0285	Latent Dirichlet Allocation
17	radon_redundant_chr	88	4595	0.0192	Multi-level linear model with varying intercept and redundant parameterization and the Choo-Hoffman parametrization
18	naive_bayes	39	4124	0.0095	Naive Bayes classifier
19	mesquite_volume	3	322	0.0093	Linear model with one transformed predictor and log transformation to measure the yield of mesquite bushes
20	cjs_t_t	22	3960	0.0056	CJS model for capture-recapture problem with parameter identifiability
21	irt_multilevel	503	90671	0.0055	Item response theory multi-level logistic model
22	irt	501	90941	0.0055	Item response theory 2-p logistic model
23	congress	4	1029	0.0039	Linear model to predict the 1988 election from 1986 election
24	dogs	3	775	0.0039	Multi-level logistic regression model for behavioral learning experiment on dogs
25	Dynocc	29	7500	0.0039	Dynamic (multi-season) site-occupancy Hidden Markov Model
26	multi_logit	32	9842	0.0033	Multinomial logistic regression
27	electric_one_pred	3	1248	0.0024	Lin. model with one predictor
28	election88	55	104094	0.0005	Multi-level logistic regression model with group level predictors to predict Republican candidate in 1988 elections
29	wells	2	15100	0.0001	Generalized linear model with logit link function and one predictor to predict shift to a safer well in Bangladesh
30	wells_dist	2	15100	0.0001	Generalized linear model with logit link function and one predictor to predict shift to a safer well in Bangladesh

Table 2: This table presents the results for ADVI baseline. ADVI runs with high variability in performance; our ADVI implementation diverges for at least 1 random trial for 10 out of 30 models.

		Full-rank Gaussian		
		ADVI		
		Closed form entropy		
		Not Used		
		1		
		1		
		ADVI Baseline		
Independent Trial		Trial 1	Trial 2	Trial 3
Id	Model Name			
1	lsat	nan	nan	nan
2	Mh	19.9685	19.9831	19.9521
3	test_simplex	-4.4433	-4.4408	-4.4373
4	endo3	-127.2903	-127.3857	-127.2958
5	gp_predict	300.0260	300.1867	300.0258
6	Mth	-152.6560	-152.6696	-152.7633
7	oxford	-4401.0033	nan	-4520.5537
8	cjs_mnl	-452.8369	-452.6761	-452.6022
9	hepatitis	-54.1560	-54.1572	-54.1076
10	normal_multi	-40367.4856	-40365.4223	-40368.5330
11	hiv_chr	nan	-74.3163	nan
12	electric_1c_chr	-287.4185	-292.0925	-286.8471
13	electric_1a_chr	-428.0037	-429.2815	-437.4855
14	electric_chr	-514.0052	-557.4496	-513.4389
15	radon_vary_si_chr	-102.4855	-102.4855	-102.5110
16	lda	-344.5263	-344.5982	-344.3087
17	radon_redundant_chr	nan	nan	-299.6408
18	naive_bayes	-3615.4987	-3615.4900	-3615.5445
19	mesquite_volume	12.4846	12.4895	nan
20	cjs_t_t	-452.8026	-452.6712	-452.5898
21	irt_multilevel	nan	nan	nan
22	irt	-15460.1601	-15460.3696	-15460.2664
23	congress	736.2241	nan	738.1187
24	dogs	-298.4544	-298.5008	-298.3045
25	Dynocc	-2126.6232	-2126.5978	-2126.6179
26	multi_logit	-554.9885	-554.6617	-554.7382
27	electric_one_pred	nan	nan	-657.4681
28	election88	-7555.5669	-7561.2245	-7556.6900
29	wells_dist	-2274.6544	nan	-2053.4626
30	wells	nan	-2041.9096	nan

Table 3: This table provides results for method that uses the closed-form entropy gradient with our comprehensive step-search scheme. We further provide *additional* the results by using Laplace Initialization scheme and using IW-sampling at inference time.

Id	Model Name	q_ϕ family												
		Step-search scheme	Full-rank Gaussian	Comprehensive step-search										
		∇_ϕ	Closed form entropy											
		LI	Not Used											
		IWVI M_{training}	Used											
		IWVI M_{sampling}	1	1									10	
		Method from Outline	(0)	10									10	
		Independent Trial	Trial 1	Trial 2	Trial 3	Additional Trial 1	Trial 2	Trial 3	Additional Trial 1	Trial 2	Trial 3	Additional Trial 1	Trial 2	Trial 3
1	lsat	-1560.3229	-1560.2861	-1560.2925	-1558.4440	-1558.3792	-1558.4386	-2666.4087	-2667.7454	-2667.5157	-2621.9313	-2622.5349	-2622.8303	
2	Mh	19.5196	19.5469	19.5496	20.4490	20.4554	20.4710	19.0324	19.0649	19.0763	20.2788	20.2878	20.2921	
3	test_simplex	-4.4463	-4.4483	-4.4402	-4.3669	-4.3745	-4.3603	-4.4438	-4.4453	-4.4496	-4.3673	-4.3731	-4.3702	
4	endo3	-127.5089	-127.5777	-127.5220	-121.1431	-121.4293	-121.2687	-127.5829	-127.6264	-127.5953	-121.3321	-121.2752	-121.4067	
5	gp_predict	198.4425	202.6357	197.5704	238.4563	238.6492	235.7607	300.0484	299.9787	300.0156	300.9871	300.9911	301.0216	
6	Mth	-153.0663	-153.0603	-153.0812	-152.3153	-152.2698	-152.3311	-153.3603	-153.3579	-153.3422	-152.4340	-152.4214	-152.4212	
7	oxford	-4333.4364	-4333.9387	-4333.7062	-4331.4304	-4331.5858	-4331.5967	-4.1115e+37	-5.9831e+44	-4.0048e+42	-1.1556e+05	-3.3595e+05	-62689.8962	
8	cjs_mnl	-452.6434	-452.6689	-452.6537	-452.0531	-452.0837	-452.0648	-452.6118	-452.6235	-452.6506	-452.0388	-452.0014	-452.0169	
9	hepatitis	-54.6239	-54.6593	-54.6598	-53.4851	-53.4839	-53.5132	-161.6031	-161.7103	-161.4679	-156.3505	-156.4540	-156.2607	
10	normal_multi	-74650.2692	-74683.3277	-74649.8184	-73234.4113	-72785.9847	-72816.0867	-16918.5887	-16918.5877	-16918.5881	-16918.5867	-16918.5857	-16918.5862	
11	hiv_chr	-74.8046	-74.7951	-74.7993	-73.6099	-73.5665	-73.6207	-74.8014	-74.8173	-74.8080	-73.6571	-73.6500	-73.6638	
12	electric_1c_chr	-285.7230	-285.8559	-286.4202	-281.1185	-281.2912	-281.4158	-285.6876	-285.9342	-286.3901	-281.1429	-281.3092	-281.3765	
13	electric_1a_chr	-424.5786	-424.5153	-424.4387	-422.3741	-422.2738	-422.1691	-424.5125	-424.4337	-424.5577	-422.3750	-422.2143	-422.3517	
14	electric_chr	-512.3681	-512.2423	-512.2471	-511.2007	-511.0951	-511.0922	-512.3493	-512.2394	-512.2689	-511.2062	-511.0864	-511.0979	
15	radon_vary_si_chr	-102.8430	-102.8273	-102.8068	-101.9041	-101.8598	-101.8806	-102.8266	-102.8438	-102.8082	-101.8498	-101.8824	-101.8779	
16	lda	-344.2642	-344.3194	-344.2521	-342.7178	-342.7799	-342.7485	-344.2697	-344.2932	-344.2646	-342.7635	-342.7396	-342.7490	
17	radon_redundant_chr	-223.6925	-225.3442	-221.3751	-218.1183	-217.9346	-217.5981	-223.5919	-467.7711	-467.6689	-218.0208	-461.9628	-461.9314	
18	naive_bayes	-3615.4642	-3615.4686	-3615.4654	-3615.1421	-3615.1434	-3615.1403	-3615.3055	-3615.3207	-3615.3055	-3615.1060	-3615.1259	-3615.1006	
19	mesquite_volume	12.4224	12.3813	12.3800	12.4977	12.5056	12.4976	12.4851	12.4834	12.4865	12.5077	12.5096	12.5132	
20	cjs_t_t	-452.6244	-452.6379	-452.6369	-452.0433	-452.0053	-452.0335	-452.6478	-452.6525	-452.6423	-452.0485	-452.0301	-452.0321	
21	irt_multilevel	-14611.3903	-14611.3943	-14611.3818	-14609.1618	-14609.1189	-14609.0938	-14608.9681	-14608.9780	-14608.9549	-14608.1255	-14608.1816	-14608.1382	
22	irt	-15427.1794	-15427.2162	-15427.1530	-15424.9416	-15424.9849	-15424.8847	-15424.2319	-15424.2349	-15424.2291	-15423.8601	-15423.8488	-15423.8540	
23	congress	738.5902	738.4774	738.4840	738.7764	738.6945	738.7785	738.7884	738.7858	738.7842	738.7941	738.7970	738.7933	
24	dogs	-298.3675	-298.2871	-298.3304	-298.2795	-298.2588	-298.2810	-298.2638	-298.2646	-298.2660	-298.2594	-298.2597	-298.2593	
25	Dynocc	-2126.6299	-2126.6223	-2126.6431	-2125.8526	-2125.8764	-2125.8708	-2126.5057	-2126.4791	-2126.4745	-2125.8125	-2125.7992	-2125.7765	
26	multi_logit	-553.8753	-553.8865	-553.8795	-553.4833	-553.4901	-553.5009	-553.5695	-553.5774	-553.5662	-553.4546	-553.4547	-553.4509	
27	electric_one_pred	-641.6253	-641.5721	-641.6571	-641.5684	-641.5582	-641.5811	-641.5624	-641.5667	-641.5647	-641.5572	-641.5598	-641.5574	
28	election88	-7534.1590	-7534.0445	-7534.1257	-7533.5235	-7533.4941	-7533.5037	-7533.6499	-7533.6635	-7533.6472	-7533.4165	-7533.4340	-7533.4334	
29	wells_dist	-2046.5482	-2046.5790	-2046.5165	-2046.5134	-2046.5195	-2046.5087	-2046.5399	-2046.5277	-2046.5413	-2046.5147	-2046.5119	-2046.5111	
30	wells	-2041.9656	-2041.9106	-2041.9605	-2041.9170	-2041.9045	-2041.9130	-2041.9045	-2041.9050	-2041.9042	-2041.9043	-2041.9044	-2041.9040	

Table 4: This table provides results for Gaussian VI that uses the “full” entropy gradient from Equation (3) with our comprehensive step-search scheme. We further provide *additional* the results when using Laplace Initialization scheme and using IW-sampling at inference time.

Id	Model Name	Full-rank Gaussian			Comprehensive step-search			Estimated without dropping score function term–full gradient			Not Used		
		Step-search scheme	Step-search scheme	Step-search scheme	Step-search scheme	Step-search scheme	Step-search scheme	Step-search scheme	Step-search scheme	Step-search scheme	Step-search scheme	Step-search scheme	Step-search scheme
		1	10	10	1	10	10	1	10	10	1	10	10
		Additional	Trial 2	Trial 3	Additional	Trial 2	Trial 3	Additional	Trial 2	Trial 3	Additional	Trial 2	Trial 3
		Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3
1	lsat	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan
2	Mh	19.0670	19.1056	19.0700	20.3383	20.3370	20.3582	19.5593	19.5481	19.5473	20.4868	20.5185	20.4844
3	test_simplex	-4.4519	-4.4444	-4.4495	-4.3659	-4.3770	-4.3691	-4.4458	-4.4436	-4.4474	-4.3599	-4.3712	-4.3588
4	endo3	-127.5600	-127.5014	-127.5194	-121.3365	-121.2019	-121.2040	-127.4403	-127.5594	-127.5994	-121.1946	-121.2420	-121.3132
5	gp_predict	300.0274	nan	299.9987	300.9504	nan	300.9560	211.0246	195.5789	204.1682	243.6565	234.2550	241.2274
6	Mth	-153.3398	-153.3258	-153.3389	-152.3910	-152.4162	-152.4159	-153.0968	-153.0545	-153.0452	-152.3186	-152.2779	-152.2451
7	oxford	-4.0948e+35	-8.6339e+39	-1.3128e+36	-1.1727e+05	-1.5272e+05	-1.3957e+05	-4333.4798	-4334.0175	-4333.8457	-4331.4394	-4331.5769	-4331.6134
8	cjs_mnl	-452.6258	-452.6614	-452.6494	-452.0289	-452.0753	-452.0496	-452.6556	-452.6672	-452.6334	-452.0531	-452.0783	-452.0089
9	hepatitis	-161.6162	-161.6264	-161.4694	-156.4100	-156.1979	-156.3142	-54.6590	-54.6527	-54.6491	-53.5409	-53.4952	-53.5208
10	normal_multi	-16918.5889	-16918.5874	-16918.5888	-16918.5869	-16918.5853	-16918.5869	-74666.1985	-74664.2850	-74649.3550	-73263.3554	-72766.8331	-72784.2473
11	hiv_chr	-74.8015	-74.7940	-74.8085	-73.6664	-73.6118	-73.6528	-74.7896	-74.8136	-74.7875	-73.6239	-73.6283	-73.5881
12	electric_1c_chr	-285.7864	-285.8934	-286.3494	-281.2761	-281.3296	-281.4412	-285.7462	-286.0667	-286.4748	-281.1279	-281.4554	-281.4536
13	electric_1a_chr	-424.4836	-424.4773	-424.5606	-422.2672	-422.2925	-422.3151	-424.4795	-424.5070	-424.4835	-422.2702	-422.2841	-422.2535
14	electric_chr	-512.3679	-512.2732	-512.2296	-511.2040	-511.1366	-511.0640	-512.3744	-512.2624	-512.2523	-511.1901	-511.1049	-511.1025
15	radon_vary_si_chr	-102.8457	-102.8146	-102.8164	-101.8595	-101.8457	-101.8769	-102.8437	-102.8427	-102.7917	-101.9166	-101.9149	-101.8222
16	lda	-344.2699	-344.2947	-344.2570	-342.7400	-342.7795	-342.7185	-344.3098	-344.3006	-344.2416	-342.7539	-342.7678	-342.7477
17	radon_redundant_chr	-467.9613	-467.9049	-467.7597	-462.4864	-462.3585	-462.1381	-223.6050	-2935.5608	-2948.1397	-218.0029	-1613.4442	-1619.0719
18	naive_bayes	-3615.3271	-3615.3214	-3615.3076	-3615.1290	-3615.1298	-3615.1107	-3615.4633	-3615.4660	-3615.4640	-3615.1420	-3615.1252	-3615.1548
19	mesquite_volume	12.4923	12.4882	12.4795	12.5160	12.5119	12.5073	12.4174	12.3694	12.3828	12.4955	12.5047	12.5044
20	cjs_t_t	-452.6280	-452.6403	-452.6759	-452.0359	-452.0043	-452.0893	-452.6438	-452.6591	-452.6367	-452.0456	-452.0408	-452.0151
21	irt_multilevel	-14608.9643	-14608.9678	-14608.9776	-14608.1555	-14608.1392	-14608.1672	-14611.3798	-14611.3839	-14611.3849	-14609.1356	-14609.0725	-14609.1173
22	irt	-15424.2420	-15424.2385	-15424.2292	-15423.8697	-15423.8673	-15423.8487	-15427.2185	-15427.1877	-15427.1430	-15424.9813	-15424.9345	-15424.9523
23	congress	738.7869	738.7817	738.7882	738.7929	738.7934	738.7973	738.6008	738.4618	738.4788	738.7810	738.6687	738.7758
24	dogs	-298.2633	-298.2652	-298.2677	-298.2589	-298.2598	-298.2612	-298.3626	-298.2907	-298.3202	-298.2743	-298.2622	-298.2661
25	Dynocc	-2126.4982	-2126.4909	-2126.5233	-2125.7935	-2125.7953	-2125.8381	-2126.6111	-2126.6211	-2126.5974	-2125.8136	-2125.8503	-2125.8062
26	multi_logit	-553.5636	-553.5538	-553.5567	-553.4501	-553.4276	-553.4351	-553.8916	-553.8986	-553.8756	-553.4952	-553.5075	-553.4867
27	electric_one_pred	-641.5643	-641.5670	-641.5643	-641.5585	-641.5605	-641.5569	-641.6257	-641.5759	-641.6568	-641.5661	-641.5609	-641.5806
28	election88	-7533.6598	-7533.6606	-7533.6501	-7533.4296	-7533.4350	-7533.4345	-7534.1616	-7534.0692	-7534.1277	-7533.5377	-7533.5224	-7533.5308
29	wells_dist	-2046.5415	-2046.5281	-2046.5470	-2046.5172	-2046.5110	-2046.5149	-2046.5478	-2046.5839	-2046.5186	-2046.5136	-2046.5238	-2046.5112
30	wells	-2041.9040	-2041.9044	-2041.9042	-2041.9038	-2041.9038	-2041.9040	-2041.9630	-2041.9106	-2041.9583	-2041.9132	-2041.9043	-2041.9110

Table 6: This table provides results for importance-weighted training for Gaussian q_ϕ optimized with our comprehensive step-search scheme. We further provide *additional* the results when using Laplace Initialization scheme and using the regular IW-ELBO gradient of Equation (5)

Id	q_ϕ family Step-search scheme ∇_ϕ LI IWVI M_{training} IWVI M_{sampling} Method from Outline Independent Trial Model Name	Full-rank Gaussian Comprehensive step-search Estimated without dropping the score-function term			Estimated with DReG			Not Used					
		Used	Not Used	Used	Not Used	Used	Not Used	Used	Not Used	Not Used			
		10	10	10	10	10	10	10	10	10	10	10	10
		Additional	Trial 2	Trial 3	Additional	Trial 2	Trial 3	Additional	Trial 2	Trial 3	Additional	Trial 2	Trial 3
		Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3
1	lsat	nan	nan	nan	nan	nan	nan	-3602.4668	-3626.9508	-3561.9721	-1560.4725	-1560.6102	-1560.2753
2	Mh	15.4818	15.7472	15.6913	19.7892	19.7846	19.8196	19.3155	19.1917	19.1727	20.7624	20.7138	20.7093
3	test_simplex	-4.3528	-4.3557	-4.3442	-4.3538	-4.3437	-4.3491	-4.3460	-4.3477	-4.3570	-4.3503	-4.3525	-4.3501
4	endo3	-121.0991	-121.1391	-121.1125	-120.9746	-121.1293	-121.0337	-120.6768	-120.6442	-120.7764	-120.7299	-120.6274	-120.7329
5	gp_predict	nan	300.6958	300.6468	300.7821	300.8882	300.7675	301.4711	301.4523	301.4776	301.5145	301.4983	nan
6	Mth	-157.6131	-157.8043	-157.8328	-152.9738	-152.8934	-152.9296	-154.0925	-154.0752	-153.8830	-152.0879	-152.0961	-152.0757
7	oxford	-1.9933e+05	-5.0506e+05	-74206.7353	-4345.0453	-4347.0228	-4346.2444	-4.9035e+05	-1.2894e+05	-37340.6443	-4344.8534	-4343.0004	-4343.6250
8	cjs_mnl	-451.8801	-451.8757	-451.8600	-451.9819	-451.9677	-451.9664	-451.8670	-451.8624	-451.8923	-451.8809	-451.8810	-451.8503
9	hepatitis	-169.5314	-170.4767	-169.9543	-69.2357	-69.3825	-70.9711	-168.6359	-168.2180	-168.8426	-55.9312	-56.1853	-56.6067
10	normal_multi	-16918.5870	-16918.5937	-16918.5867	-26750.2857	-27498.9976	-27460.3790	-16918.5864	-16918.5864	-16918.5863	-27788.4873	-26875.6551	-27865.8058
11	hiv_chr	-176.5920	-175.6895	-171.8587	-74.9593	-74.9456	-75.1526	-174.1049	-170.4290	-170.1433	-73.5738	-73.5807	-73.6530
12	electric_1c_chr	-286.7872	-287.3433	-286.7932	-315.0138	-313.2617	-315.6589	-285.7240	-286.3400	-284.3945	-310.0764	-314.5847	-311.5810
13	electric_1a_chr	-426.9384	-426.9405	-428.7423	-426.9211	-428.3849	-428.2209	-422.5884	-426.4747	-430.4513	-422.5316	-422.7934	-423.0203
14	electric_chr	-516.2415	-516.4791	-516.0333	-516.2482	-516.6440	-515.8745	-515.7389	-515.3542	-514.7078	-515.9188	-515.7946	-515.8023
15	radon_vary_si_chr	-103.8548	-104.1821	-103.7281	-102.8569	-102.9285	-102.9329	-178.6936	-181.2776	-175.7665	-101.6374	-101.6283	-101.6344
16	lda	-342.3627	-342.3805	-342.3895	-342.4098	-342.3976	-342.4005	-342.3420	-342.3486	-342.2886	-342.3074	-342.3318	-342.3201
17	radon_redundant_chr	-356.7974	-453.5837	-358.3671	-693.8210	-693.9595	-3186.8453	-449.6303	-449.8883	-452.8245	-671.9259	-691.9953	-3202.9959
18	naive_bayes	-3615.0965	-3615.1078	-3615.0916	-3615.3434	-3615.3476	-3615.3793	-3615.0964	-3615.1020	-3615.1063	-3615.1163	-3615.0989	-3615.0960
19	mesquite_volume	12.5129	12.5125	12.5134	12.3802	12.3888	12.2544	12.5120	12.5108	12.5123	12.5071	12.5101	12.5141
20	cjs_t_t	-451.8701	-451.8341	-451.8730	-452.0175	-451.9672	-452.0109	-451.9038	-451.8530	-451.8859	-451.8573	-451.8625	-451.8934
21	irt_multilevel	-14609.2097	-14609.3464	-14608.4966	-14622.5119	-14622.2421	-14622.6026	-14607.9892	-14608.0042	-14608.0028	-14611.7850	-14611.8132	-14611.5983
22	irt	-15423.9092	-15423.9159	-15423.9325	-15437.7767	-15437.2800	-15437.1353	-15423.8471	-15423.8396	-15423.8208	-15424.2517	-15423.9661	-15427.9253
23	congress	738.7864	738.7833	738.7801	738.6621	738.5947	738.6958	738.7922	738.7937	738.7952	738.7948	738.7948	738.7956
24	dogs	-298.2718	-298.2617	-298.2698	-298.4308	-298.4959	-298.3189	-298.2585	-298.2587	-298.2598	-298.2605	-298.2574	-298.2614
25	Dynocc	-2125.6550	-2125.6638	-2125.7156	-2125.8873	-2125.9113	-2125.8858	-2125.6986	-2125.6466	-2125.5890	-2125.6676	-2125.6854	-2125.6376
26	multi_logit	-553.5210	-553.5132	-553.4919	-554.1409	-553.8148	-554.0896	-553.4295	-553.4241	-553.4322	-553.4322	-553.4350	-553.4397
27	electric_one_pred	-641.5591	-641.5585	-641.5581	-641.9277	-641.7308	-641.6937	-641.5579	-641.5594	-641.5546	-641.5589	-641.5605	-641.5588
28	election88	-7533.4531	-7533.4451	-7533.4654	-7534.4716	-7534.6690	-7534.5011	-7533.4137	-7533.4106	-7533.4142	-7533.4076	-7533.4078	-7533.4052
29	wells_dist	-2046.5308	-2046.5357	-2046.5255	-2046.6939	-2046.5931	-2046.5876	-2046.5091	-2046.5093	-2046.5089	-2046.5092	-2046.5090	-2046.5089
30	wells	-2041.9053	-2041.9222	-2041.9059	-2042.0735	-2041.9343	-2042.0528	-2041.9041	-2041.9040	-2041.9039	-2041.9040	-2041.9039	-2041.9039

Table 7: This table provides results for real-NVP normalizing flows optimized with our comprehensive step-search scheme with additional results from using IW-sampling.

Id	Model Name	Real NVP flows										Estimated with STL		
		Comprehensive step-search										Not Used		
		Estimated without dropping the score-function term–full gradient										Not Used		
		Not Used										Not Used		
		1										1		
		10										10		
		Additional										(4c)		
		(4a)										(4b)		
		Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3	
1	lsat	-1558.0810	-1558.0983	-1558.0795	-1557.4331	-1557.4355	-1557.4532	-1557.7891	-1557.7745	-1557.7618	-1557.3710	-1557.3581	-1557.3378	
2	Mh	20.6116	20.6099	20.5906	21.0692	21.0748	21.0498	20.8141	20.7952	20.7906	21.1431	21.1399	21.1405	
3	test_simplex	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	
4	endo3	-125.4364	-125.6489	-125.3696	-119.9958	-120.1006	-119.8449	-124.1439	-124.6179	-123.8879	-119.0637	-119.4145	-118.8396	
5	gp_predict	301.0234	300.9385	133.3838	301.8497	301.8672	175.2945	291.8903	186.8792	278.3282	295.9186	222.9463	287.6078	
6	Mth	-152.0877	-152.1042	-152.0981	-151.8264	-151.8418	-151.8434	-151.9116	-151.8974	-151.9065	-151.7999	-151.7864	-151.7871	
7	oxford	-4332.3919	-4332.4422	-4332.3601	-4331.2495	-4331.2409	-4331.2086	-4331.7142	-4331.7552	-4331.6724	-4330.9652	-4330.9303	-4330.9149	
8	cjs_mnl	-451.6828	-451.6553	-451.7014	-451.5297	-451.5138	-451.5268	-451.5370	-451.5515	-451.5312	-451.5047	-451.5007	-451.5000	
9	hepatitis	-52.1719	-52.0280	-51.9546	-51.3164	-51.2786	-51.1834	-51.1649	-51.1504	-51.0317	-50.8315	-50.7965	-50.7713	
10	normal_multi	-16937.4055	-16924.0775	-16940.7436	-16930.1828	-16920.9157	-16930.9541	-16919.3660	-16933.2347	-16919.2307	-16918.7303	-16926.7185	-16918.7138	
11	hiv_chr	-74.0555	-74.4123	-74.2517	-73.0828	-73.2133	-73.1843	-73.1723	-73.0908	-73.1615	-72.8201	-72.7956	-72.8215	
12	electric_1c_chr	-279.5105	-279.2506	-278.9096	-278.1362	-278.0216	-277.9078	-278.1784	-278.8128	-278.2789	-277.6591	-277.8439	-277.6683	
13	electric_1a_chr	-420.8645	-420.9422	-420.8577	-420.2430	-420.2319	-420.2248	-420.2447	-420.3372	-420.2873	-420.0749	-420.1021	-420.0974	
14	electric_chr	-510.9007	-510.8399	-511.0042	-510.6317	-510.6201	-510.6661	-510.6236	-510.6386	-510.6629	-510.6001	-510.6022	-510.6002	
15	radon_vary_si_chr	-102.3573	-102.2121	-102.0270	-101.5372	-101.5044	-101.4406	-101.4443	-101.5437	-101.4984	-101.3241	-101.3366	-101.3272	
16	lda	nan	-343.8487	nan	nan	-342.5254	nan	nan	nan	nan	nan	nan	nan	
17	radon_redundant_chr	-217.3711	-217.2081	-217.2531	-216.9475	-216.9049	-216.9103	-216.9012	-217.0216	-216.9071	-216.8625	-216.8828	-216.8627	
18	naive_bayes	-3615.3514	-3615.2491	-3615.3346	-3615.1268	-3615.1000	-3615.1178	-3615.0951	-3615.1031	-3615.1061	-3615.0718	-3615.0772	-3615.0768	
19	mesquite_volume	12.4818	12.4943	12.4949	12.5128	12.5150	12.5175	12.5073	12.4761	12.5053	12.5132	12.5085	12.5139	
20	cjs_t_t	-451.6751	-451.6590	-451.6910	-451.5173	-451.5230	-451.5276	-451.5337	-451.5676	-451.5380	-451.5010	-451.5019	-451.5029	
21	irt_multilevel	-14609.0529	-14609.1944	-14609.0893	-14608.1901	-14608.2447	-14608.2274	-14608.3838	-14608.3419	-14608.3424	-14608.0398	-14608.0113	-14608.0313	
22	irt	-15425.1807	-15425.0129	-15424.9788	-15424.1654	-15424.0792	-15424.0399	-15424.3563	-15424.2689	-15424.2745	-15423.8821	-15423.8861	-15423.8640	
23	congress	738.7674	738.6810	738.4917	738.7953	738.7737	738.7619	738.6337	738.7920	738.5114	738.7762	738.7957	738.7648	
24	dogs	-298.3447	-303.0714	-298.2653	-298.2672	-302.1189	-298.2595	-298.2593	-298.2587	-298.2587	-298.2587	-298.2580	-298.2578	
25	Dynocc	-2125.4343	-2125.4809	-2125.4959	-2125.1858	-2125.2057	-2125.2117	-2125.2266	-2125.2430	-2125.2304	-2125.1621	-2125.1556	-2125.1584	
26	multi_logit	-554.3855	-554.2881	-554.4112	-553.6644	-553.6392	-553.6909	-553.8005	-553.8478	-553.8052	-553.4846	-553.5251	-553.4879	
27	electric_one_pred	-641.6955	-641.5924	-641.7577	-641.5716	-641.5595	-641.5836	-641.5577	-641.5823	-641.5729	-641.5568	-641.5594	-641.5580	
28	election88	-7533.5399	-7533.5842	-7533.6034	-7533.4097	-7533.4182	-7533.4205	-7533.4139	-7533.3991	-7533.4044	-7533.3948	-7533.3908	-7533.3919	
29	wells_dist	-14358.7734	-2053.1972	-2066.2398	-2107.7104	-2052.5297	-2052.9980	-2046.5242	-2046.5117	-2046.5132	-2046.5109	-2046.5098	-2046.5107	
30	wells	-2053.2450	-2128.8088	-2043.5417	-2052.6375	-2057.4116	-2043.0341	-2041.9040	-2041.9045	-2041.9038	-2041.9039	-2041.9043	-2041.9037	

Table 8: This table provides results for importance weighted training for real-NVP normalizing flows optimized with our comprehensive step-search scheme with additional results from using regular IW-ELBO gradient.

Id	q_ϕ family Step-search scheme ∇_ϕ LI IWVI M_{training} IWVI M_{sampling} Method from Outline Independent Trial Model Name	Real NVP flows Comprehensive step-search					
		Estimated w/o dropping score-function term			Estimated with DReG		
		Not Used		Not Used			
		10		10			
		10		10			
		Additional			(4d)		
		Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3
1	lsat	-1557.7324	-1557.7093	-1557.7707	-1557.3724	-1557.3555	-1557.3413
2	Mh	20.8262	20.8106	20.8031	21.1380	21.1331	21.1265
3	test_simplex	nan	nan	nan	nan	nan	nan
4	endo3	-120.3320	-120.4250	-120.4874	-120.0272	-119.9676	-120.1827
5	gp_predict	300.1498	300.0910	300.6795	301.7336	301.7699	301.7164
6	Mth	-151.9868	-152.0086	-152.0120	-151.8052	-151.7779	-151.8100
7	oxford	-4332.1323	-4332.3033	-4332.4134	-4331.0128	-4331.0230	-4330.9522
8	cjs_mnl	-451.7348	-451.7418	-451.7667	-451.5060	-451.5204	-451.5041
9	hepatitis	-52.2705	-52.4800	-52.5429	-50.8712	-51.2069	-50.8934
10	normal_multi	-16933.1393	-16940.4390	-16935.3070	-16920.0900	-16922.8421	-16937.6249
11	hiv_chr	-74.9543	-75.1996	-75.2645	-73.0401	-72.9434	-72.8453
12	electric_1c_chr	-279.7025	-279.6760	-279.8671	-278.0520	-278.2926	-278.3740
13	electric_1a_chr	-421.0590	-421.0157	-421.1706	-420.1473	-420.1479	-420.1098
14	electric_chr	-510.8465	-511.4763	-510.9585	-510.6169	-510.6045	-510.6419
15	radon_vary_si_chr	-102.8107	-102.1768	-102.3642	-101.6430	-101.3792	-101.3284
16	lda	-342.2148	-342.1463	-341.9619	-342.1034	nan	-342.1726
17	radon_redundant_chr	-217.5033	-217.3719	-217.3199	-219.1729	-216.8761	-216.8774
18	naive_bayes	-3615.2138	-3615.1675	-3615.2120	-3615.0806	-3615.0806	-3615.0849
19	mesquite_volume	12.4558	12.4775	12.4488	12.4897	12.5151	12.5162
20	cjs_t_t	-451.6491	-451.6962	-451.7152	-451.7311	-451.5933	-451.5014
21	irt_multilevel	-14609.2872	-14609.3237	-14609.3317	-14608.0970	-14608.0508	-14608.0362
22	irt	-15424.9266	-15425.1680	-15424.9245	-15423.8881	-15423.9093	-15423.9310
23	congress	738.7386	738.7660	738.7162	738.7869	738.7954	738.7907
24	dogs	-298.3505	-298.2761	-298.2739	-298.2580	-298.2586	-298.2581
25	Dynocc	-2125.3477	-2125.3606	-2125.3213	-2125.1688	-2125.1674	-2125.1792
26	multi_logit	-555.2918	-556.6276	-555.3734	-556.2806	-553.5680	-554.7593
27	electric_one_pred	-641.6248	-641.5941	-641.6119	-641.5573	-641.5567	-641.5628
28	election88	-7533.5460	-7533.6522	-7533.6817	-7533.3927	-7533.4052	-7533.3914
29	wells_dist	-2046.7589	-2057.7702	-2046.6208	-2046.5093	-2046.5150	-2046.5097
30	wells	-2047.6023	-2041.9124	-2041.9151	-2041.9042	-2041.9042	-2041.9038

Table 9: This table presents the results for additional Diagonal Gaussian experiments. Please refer to [Figure 11](#) and [appendix B](#) for more details.

Id	Model Name	Diagonal Gaussian								
		Comprehensive step-search			Estimated with STL			10		
q_ϕ family	Step-search scheme	Closed form entropy			Not Used			Additional		
∇_ϕ	LI	Not Used			Not Used			Additional		
IWVI M_{training}	IWVI M_{sampling}	1			1			10		
Method from Outline	Independent Trial	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3
1	lsat	-1593.5322	-1593.4869	-1593.3559	-1592.8262	-1592.4748	-1592.5821	-1571.0762	-1570.9308	-1570.8328
2	Mh	19.1775	19.1667	19.1541	19.1718	19.1684	19.1918	19.9559	19.9322	19.9619
3	test_simplex	-4.4521	-4.4428	-4.4479	-4.4365	-4.4451	-4.4432	-4.3572	-4.3665	-4.3664
4	endo3	-128.4125	-128.4300	-128.4104	-128.3513	-128.4653	-128.3904	-122.0453	-122.1725	-122.1298
5	gp_predict	125.4957	124.4540	109.7607	119.1200	113.7045	126.2959	173.3857	170.0907	178.5877
6	Mth	-153.1179	-153.1375	-153.1227	-153.1145	-153.0937	-153.1330	-152.5015	-152.5002	-152.5632
7	oxford	-4351.8876	-4352.1289	-4352.0302	-4351.8651	-4351.9882	-4352.0168	-4334.3600	-4334.3489	-4334.3732
8	cjs_mnl	-455.1820	-455.1343	-455.1980	-455.1473	-455.1559	-455.1645	-453.5222	-453.4747	-453.5459
9	hepatitis	-56.9566	-56.9034	-56.9102	-56.7279	-56.7292	-56.7131	-55.1387	-55.1739	-55.1519
10	normal_multi	-74651.8168	-74653.5847	-74651.7663	-74651.0597	-74657.3869	-74653.1409	-74006.7030	-74007.7665	-73999.5017
11	hiv_chr	-88.0622	-88.1118	-88.0928	-88.0838	-88.1383	-88.1089	-86.3650	-86.4350	-86.3553
12	electric_1c_chr	-293.8758	-293.8000	-293.7533	-293.8438	-293.7498	-293.8464	-289.9068	-289.8101	-289.8923
13	electric_1a_chr	-427.1647	-427.1551	-427.1726	-427.1397	-427.1230	-427.1873	-424.2745	-424.2433	-424.3046
14	electric_chr	-513.1907	-513.1651	-513.1779	-513.1541	-513.1480	-513.1572	-512.1036	-512.1022	-512.0917
15	radon_vary_si_chr	-105.8260	-105.8688	-105.8414	-105.8406	-105.8733	-105.8842	-103.5692	-103.6337	-103.6410
16	lda	-344.4616	-344.4580	-344.4734	-344.4943	-344.5078	-344.4530	-342.8903	-342.8522	-342.8561
17	radon_redundant_chr	-218.1631	-218.2137	-218.2104	-218.1262	-218.2738	-218.1381	-217.4305	-217.4860	-217.5006
18	naive_bayes	-3615.2682	-3615.2812	-3615.2838	-3615.2553	-3615.2565	-3615.2691	-3615.1094	-3615.1041	-3615.1181
19	mesquite_volume	12.1762	12.1763	12.1197	12.1633	12.1528	12.1737	12.4216	12.4033	12.4035
20	cjs_t_t	-455.1950	-455.1641	-455.2009	-455.1728	-455.1777	-455.1742	-453.4716	-453.5388	-453.5097
21	irt_multilevel	-14631.4012	-14632.0799	-14631.5253	-14631.2708	-14631.9146	-14631.2243	-14611.8698	-14611.8590	-14611.7534
22	irt	-15443.3924	-15443.1456	-15443.8044	-15443.3331	-15443.2550	-15443.4153	-15426.3968	-15426.4443	-15426.4066
23	congress	737.0282	736.7399	736.9055	737.0364	736.8671	736.7321	737.5111	737.4481	737.5068
24	dogs	-299.3324	-299.3696	-299.3739	-299.3697	-299.4016	-299.3477	-298.7402	-298.7262	-298.7594
25	Dynocc	-2129.9383	-2129.9050	-2129.8542	-2129.8750	-2129.8567	-2129.9244	-2127.8466	-2127.7597	-2127.8208
26	multi_logit	-575.8037	-575.8263	-575.8159	-575.8136	-575.7877	-575.8724	-572.5463	-572.5639	-572.6479
27	electric_one_pred	-641.9286	-641.9152	-641.9057	-641.9139	-641.9218	-641.9175	-641.6821	-641.6903	-641.6910
28	election88	-7534.3065	-7534.3075	-7534.3145	-7534.2861	-7534.2890	-7534.2778	-7533.7389	-7533.7166	-7533.7257
29	wells_dist	-2047.2697	-2047.0170	-2048.8710	-2047.2355	-2047.0116	-2047.2456	-2046.7341	-2046.7397	-2046.7401
30	wells	-2042.4365	-2042.4200	-2042.3901	-2042.4154	-2042.4080	-2042.4133	-2042.1239	-2042.1286	-2042.0731

I Complete table for per iteration training times

For completeness, we include the per iterations training times of all the VI methods we experiment with. However, these training times should be read into with caution. We interface with Pystan and Autograd for our work; this creates an extra overhead with can dominate the run-times when the models are expensive to evaluate. Further, each training instance is run on a single CPU core.

Table 10: This table presents the per iteration training times for ADVI baseline. Please refer to [Table 2](#) for lower-bound results.

		Full-rank Gaussian		
		ADVI		
		Closed form entropy		
		Not Used		
		1		
		1		
		Trial 1	Trial 2	Trial 3
Id	Model Name			
1	lsat	0.2802	0.2805	0.2800
2	Mh	0.1252	0.1294	0.1234
3	test_simplex	0.0158	0.0169	0.0154
4	endo3	0.0450	0.0453	0.0458
5	gp_predict	1.3203	1.2598	1.2821
6	Mth	0.1207	0.1061	0.1069
7	oxford	0.0585	0.0582	0.0581
8	cjs_mnl	0.0242	0.0206	0.0236
9	hepatitis	0.0451	0.0456	0.0455
10	normal_multi	0.2398	0.2392	0.2391
11	hiv_chr	0.0422	0.0426	0.0429
12	electric_1c_chr	0.0256	0.0272	0.0254
13	electric_1a_chr	0.0361	0.0391	0.0372
14	electric_chr	0.0243	0.0262	0.0254
15	radon_vary_si_chr	0.0477	0.0476	0.0475
16	lda	0.0447	0.0518	0.0510
17	radon_redundant_chr	0.0235	0.0235	0.0236
18	naive_bayes	0.1284	0.1280	0.1282
19	mesquite_volume	0.0163	0.0162	0.0163
20	cjs_t_t	0.1104	0.1102	0.1044
21	irt_multilevel	0.7842	0.7865	0.7845
22	irt	0.8777	0.8527	0.8809
23	congress	0.0223	0.0196	0.0224
24	dogs	0.0440	0.0440	0.0440
25	Dynocc	0.1484	0.1423	0.1420
26	multi_logit	0.1109	0.1070	0.1076
27	electric_one_pred	0.0179	0.0179	0.0178
28	election88	0.3556	0.3510	0.3512
29	wells_dist	0.0768	0.0769	0.0792
30	wells	0.0914	0.0932	0.0827

Table 11: This table provides the per iteration training times for method that uses the closed-form entropy gradient with our comprehensive step-search scheme. Refer to Table 3 for lower-bound results.

Id	Model Name	q_ϕ family	Step-search scheme	∇_ϕ	LI	Full-rank Gaussian											
						Comprehensive step-search			Closed form entropy			Used					
	Independent Trial					1	10	1	10	1	10	1	10	1	10		
						Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3	Trial 3		
1	lsat					0.3344	0.1938	0.3348	0.3344	0.1938	0.3348	0.3297	0.3278	0.3299	0.3297	0.3278	0.3299
2	Mh					0.0834	0.0949	0.0954	0.0834	0.0949	0.0954	0.0939	0.0925	0.0926	0.0939	0.0925	0.0926
3	test_simplex					0.0215	0.0212	0.0223	0.0215	0.0212	0.0223	0.0191	0.0208	0.0212	0.0191	0.0208	0.0212
4	endo3					0.0292	0.0290	0.0290	0.0292	0.0290	0.0290	0.0291	0.0261	0.0291	0.0291	0.0261	0.0291
5	gp_predict					1.1382	1.1475	1.1472	1.1382	1.1475	1.1472	1.0495	1.0156	0.9774	1.0495	1.0156	0.9774
6	Mth					0.0898	0.0890	0.0890	0.0898	0.0890	0.0890	0.0876	0.0924	0.0881	0.0876	0.0924	0.0881
7	oxford					0.0340	0.0321	0.0319	0.0340	0.0321	0.0319	0.0365	0.0304	0.0366	0.0365	0.0304	0.0366
8	cjs_mnl					0.0277	0.0259	0.0281	0.0277	0.0259	0.0281	0.0210	0.0217	0.0217	0.0210	0.0217	0.0217
9	hepatitis					0.0315	0.0284	0.0282	0.0315	0.0284	0.0282	0.0299	0.0277	0.0279	0.0299	0.0277	0.0279
10	normal_multi					0.1459	0.1441	0.1450	0.1459	0.1441	0.1450	0.1350	0.1356	0.1346	0.1350	0.1356	0.1346
11	hiv_chr					0.0282	0.0279	0.0284	0.0282	0.0279	0.0284	0.0277	0.0304	0.0280	0.0277	0.0304	0.0280
12	electric_1c_chr					0.0263	0.0244	0.0262	0.0263	0.0244	0.0262	0.0246	0.0261	0.0245	0.0246	0.0261	0.0245
13	electric_1a_chr					0.0250	0.0247	0.0249	0.0250	0.0247	0.0249	0.0244	0.0353	0.0242	0.0244	0.0353	0.0242
14	electric_chr					0.0215	0.0215	0.0215	0.0215	0.0215	0.0215	0.0218	0.0218	0.0217	0.0218	0.0218	0.0217
15	radon_vary_si_chr					0.0292	0.0293	0.0307	0.0292	0.0293	0.0307	0.0259	0.0309	0.0309	0.0259	0.0309	0.0309
16	lda					0.0387	0.0398	0.0400	0.0387	0.0398	0.0400	0.0398	0.0356	0.0355	0.0398	0.0356	0.0355
17	radon_redundant_chr					0.0221	0.0211	0.0213	0.0221	0.0211	0.0213	0.0213	0.0219	0.0192	0.0213	0.0219	0.0192
18	naive_bayes					0.0734	0.0757	0.0732	0.0734	0.0757	0.0732	0.0844	0.0820	0.0820	0.0844	0.0820	0.0820
19	mesquite_volume					0.0141	0.0145	0.0142	0.0141	0.0145	0.0142	0.0145	0.0144	0.0145	0.0145	0.0144	0.0145
20	cjs_t					0.0679	0.0852	0.0850	0.0679	0.0852	0.0850	0.0852	0.0748	0.0755	0.0852	0.0748	0.0755
21	irt_multilevel					0.7569	0.7563	0.7526	0.7569	0.7563	0.7526	0.9201	0.9183	0.9202	0.9201	0.9183	0.9202
22	irt					0.9308	0.9239	0.9264	0.9308	0.9239	0.9264	0.9238	0.8785	0.5136	0.9238	0.8785	0.5136
23	congress					0.0177	0.0178	0.0177	0.0177	0.0178	0.0177	0.0176	0.0176	0.0175	0.0176	0.0176	0.0175
24	dogs					0.0314	0.0338	0.0316	0.0314	0.0338	0.0316	0.0357	0.0356	0.0355	0.0357	0.0356	0.0355
25	Dynocc					0.1006	0.1156	0.1011	0.1006	0.1156	0.1011	0.1165	0.0962	0.1161	0.1165	0.0962	0.1161
26	multi_logit					0.0792	0.0792	0.0789	0.0792	0.0792	0.0789	0.0819	0.0819	0.0819	0.0819	0.0819	0.0819
27	electric_one_pred					0.0229	0.0197	0.0197	0.0229	0.0197	0.0197	0.0220	0.0181	0.0223	0.0220	0.0181	0.0223
28	election88					0.2555	0.2544	0.2548	0.2555	0.2544	0.2548	0.2474	0.2267	0.2471	0.2474	0.2267	0.2471
29	wells_dist					0.0557	0.0558	0.0558	0.0557	0.0558	0.0558	0.0578	0.0774	0.0572	0.0578	0.0774	0.0572
30	wells					0.0672	0.0660	0.0662	0.0672	0.0660	0.0662	0.0667	0.0655	0.0658	0.0667	0.0655	0.0658

Table 12: This table provides per iteration training times for Gaussian VI that uses the “full” entropy gradient from Equation (3) with our comprehensive step-search scheme. Refer to Table 4 for lower-bound results.

Id	q_ϕ family	Full-rank Gaussian											
		Comprehensive step-search						Estimated without dropping score function term—full gradient					
	Step-search scheme	Used			Not Used			Used			Not Used		
	∇_ϕ	1			10			1			10		
	LI	1			10			1			10		
	IWVI M_{training}	1			10			1			10		
	IWVI M_{sampling}	1			10			1			10		
	Independent Trial	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3
	Model Name												
1	lsat	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan
2	Mh	0.2940	0.3405	0.3059	0.2940	0.3405	0.3059	0.3256	0.3022	0.3277	0.3256	0.3022	0.3277
3	test_simplex	0.0188	0.0211	0.0208	0.0188	0.0211	0.0208	0.0207	0.0188	0.0215	0.0207	0.0188	0.0215
4	endo3	0.0630	0.0652	0.0634	0.0630	0.0652	0.0634	0.0630	0.0672	0.0632	0.0630	0.0672	0.0632
5	gp_predict	1.1061	nan	1.0685	1.1061	nan	1.0685	0.9109	1.0880	1.0933	0.9109	1.0880	1.0933
6	Mth	0.2856	0.2957	0.3500	0.2856	0.2957	0.3500	0.2951	0.3391	0.3362	0.2951	0.3391	0.3362
7	oxford	0.1088	0.1041	0.1273	0.1088	0.1041	0.1273	0.1109	0.1096	0.1087	0.1109	0.1096	0.1087
8	cjs_mnl	0.0272	0.0287	0.0276	0.0272	0.0287	0.0276	0.0268	0.0277	0.0286	0.0268	0.0277	0.0286
9	hepatitis	0.0931	0.0987	0.0986	0.0931	0.0987	0.0986	0.0894	0.0993	0.0990	0.0894	0.0993	0.0990
10	normal_multi	0.1769	0.1776	0.1776	0.1769	0.1776	0.1776	0.1783	0.1756	0.1772	0.1783	0.1756	0.1772
11	hiv_chr	0.0626	0.0632	0.0610	0.0626	0.0632	0.0610	0.0611	0.0609	0.0593	0.0611	0.0609	0.0593
12	electric_1c_chr	0.0424	0.0413	0.0424	0.0424	0.0413	0.0424	0.0425	0.0430	0.0427	0.0425	0.0430	0.0427
13	electric_1a_chr	0.0394	0.0396	0.0404	0.0394	0.0396	0.0404	0.0397	0.0409	0.0407	0.0397	0.0409	0.0407
14	electric_chr	0.0352	0.0360	0.0343	0.0352	0.0360	0.0343	0.0350	0.0357	0.0357	0.0350	0.0357	0.0357
15	radon_vary_si_chr	0.0642	0.0584	0.0640	0.0642	0.0584	0.0640	0.0629	0.0642	0.0650	0.0629	0.0642	0.0650
16	lda	0.0488	0.0492	0.0491	0.0488	0.0492	0.0491	0.0489	0.0486	0.0491	0.0489	0.0486	0.0491
17	radon_redundant_chr	0.0349	0.0343	0.0340	0.0349	0.0343	0.0340	0.0343	0.0343	0.0343	0.0343	0.0343	0.0343
18	naive_bayes	0.0941	0.0948	0.0955	0.0941	0.0948	0.0955	0.0953	0.0967	0.0962	0.0953	0.0967	0.0962
19	mesquite_volume	0.0206	0.0209	0.0208	0.0206	0.0209	0.0208	0.0194	0.0223	0.0198	0.0194	0.0223	0.0198
20	cjs_t_t	0.1015	0.0981	0.1015	0.1015	0.0981	0.1015	0.0960	0.0967	0.0978	0.0960	0.0967	0.0978
21	irt_multilevel	1.3379	0.9867	1.0794	1.3379	0.9867	1.0794	1.0716	0.9969	1.1124	1.0716	0.9969	1.1124
22	irt	1.1066	1.0423	0.9769	1.1066	1.0423	0.9769	1.1529	1.0222	1.0689	1.1529	1.0222	1.0689
23	congress	0.0277	0.0271	0.0272	0.0277	0.0271	0.0272	0.0273	0.0271	0.0280	0.0273	0.0271	0.0280
24	dogs	0.0454	0.0430	0.0447	0.0454	0.0430	0.0447	0.0436	0.0451	0.0447	0.0436	0.0451	0.0447
25	Dynocc	0.1224	0.1229	0.1329	0.1224	0.1229	0.1329	0.1212	0.1203	0.1209	0.1212	0.1203	0.1209
26	multi_logit	0.0981	0.0967	0.0964	0.0981	0.0967	0.0964	0.0982	0.0984	0.1002	0.0982	0.0984	0.1002
27	electric_one_pred	0.0209	0.0207	0.0213	0.0209	0.0207	0.0213	0.0206	0.0210	0.0212	0.0206	0.0210	0.0212
28	election88	0.2777	0.2732	0.2747	0.2777	0.2732	0.2747	0.2398	0.2817	0.2668	0.2398	0.2817	0.2668
29	wells_dist	0.0753	0.0757	0.0775	0.0753	0.0757	0.0775	0.0765	0.0754	0.0759	0.0765	0.0754	0.0759
30	wells	0.0828	0.0819	0.0813	0.0828	0.0819	0.0813	0.0823	0.0816	0.0812	0.0823	0.0816	0.0812

Table 13: This table provides per iteration training times when using STL gradient from Equation (3) with our comprehensive step-search scheme. Please refer to Table 5 for lower-bound results.

Id	Model Name	q_ϕ family			Full-rank Gaussian			Step-search scheme			Comprehensive step-search		
		∇_ϕ	LI	Used	Used	Not Used	Used	Not Used	Used	Not Used	Used	Not Used	
		1	10	10	1	10	10	1	10	10	1	10	
		Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3
1	lsat	0.6813	0.6598	0.8223	0.6813	0.6598	0.8223	0.6002	0.9192	0.6543	0.6002	0.9192	0.6543
2	Mh	0.1398	0.1327	0.1330	0.1398	0.1327	0.1330	0.1295	0.1345	0.1340	0.1295	0.1345	0.1340
3	test_simplex	0.0191	0.0141	0.0129	0.0191	0.0141	0.0129	0.0213	0.0136	0.0259	0.0213	0.0136	0.0259
4	endo3	0.0443	0.0315	0.0322	0.0443	0.0315	0.0322	0.0446	0.0310	0.0390	0.0446	0.0310	0.0390
5	gp_predict	1.1767	0.9317	0.8194	1.1767	0.9317	0.8194	1.1775	0.8208	1.1216	1.1775	0.8208	1.1216
6	Mth	0.1394	0.1194	0.1185	0.1394	0.1194	0.1185	0.1410	0.1418	0.1235	0.1410	0.1418	0.1235
7	oxford	0.0618	0.0486	0.0518	0.0618	0.0486	0.0518	0.0651	0.0527	0.0511	0.0651	0.0527	0.0511
8	cjs_mnl	0.0273	0.0210	0.0211	0.0273	0.0210	0.0211	0.0288	0.0210	0.0198	0.0288	0.0210	0.0198
9	hepatitis	0.0515	0.0500	0.0394	0.0515	0.0500	0.0394	0.0504	0.0416	0.0418	0.0504	0.0416	0.0418
10	normal_multi	0.1713	0.1477	0.1375	0.1713	0.1477	0.1375	0.1746	0.1475	0.1475	0.1746	0.1475	0.1475
11	hiv_chr	0.0319	0.0350	0.0352	0.0319	0.0350	0.0352	0.0421	0.0352	0.0348	0.0421	0.0352	0.0348
12	electric_1c_chr	0.0355	0.0283	0.0284	0.0355	0.0283	0.0284	0.0356	0.0283	0.0297	0.0356	0.0283	0.0297
13	electric_1a_chr	0.0323	0.0289	0.0271	0.0323	0.0289	0.0271	0.0330	0.0273	0.0289	0.0330	0.0273	0.0289
14	electric_chr	0.0299	0.0240	0.0244	0.0299	0.0240	0.0244	0.0304	0.0258	0.0245	0.0304	0.0258	0.0245
15	radon_vary_si_chr	0.0463	0.0377	0.0376	0.0463	0.0377	0.0376	0.0455	0.0373	0.0373	0.0455	0.0373	0.0373
16	lda	0.0478	0.0503	0.0495	0.0478	0.0503	0.0495	0.0479	0.0405	0.0406	0.0479	0.0405	0.0406
17	radon_redundant_chr	0.0308	0.0244	0.0241	0.0308	0.0244	0.0241	0.0308	0.0246	0.0245	0.0308	0.0246	0.0245
18	naive_bayes	0.0960	0.0855	0.0863	0.0960	0.0855	0.0863	0.0953	0.0762	0.0716	0.0953	0.0762	0.0716
19	mesquite_volume	0.0196	0.0145	0.0144	0.0196	0.0145	0.0144	0.0207	0.0145	0.0207	0.0207	0.0145	0.0207
20	cjs_t_t	0.0958	0.0821	0.0849	0.0958	0.0821	0.0849	0.0926	0.0845	0.0779	0.0926	0.0845	0.0779
21	irt_multilevel	0.8995	1.1413	1.1138	0.8995	1.1413	1.1138	0.8913	0.9329	0.7391	0.8913	0.9329	0.7391
22	irt	0.9916	0.6671	0.7762	0.9916	0.6671	0.7762	0.9206	0.7895	0.7731	0.9206	0.7895	0.7731
23	congress	0.0269	0.0183	0.0179	0.0269	0.0183	0.0179	0.0264	0.0179	0.0180	0.0264	0.0179	0.0180
24	dogs	0.0439	0.0369	0.0367	0.0439	0.0369	0.0367	0.0456	0.0367	0.0370	0.0456	0.0367	0.0370
25	Dynocc	0.1260	0.1156	0.1159	0.1260	0.1156	0.1159	0.1273	0.1155	0.1060	0.1273	0.1155	0.1060
26	multi_logit	0.0977	0.0822	0.0852	0.0977	0.0822	0.0852	0.0983	0.0842	0.0829	0.0983	0.0842	0.0829
27	electric_one_pred	0.0214	0.0146	0.0147	0.0214	0.0146	0.0147	0.0226	0.0155	0.0154	0.0226	0.0155	0.0154
28	election88	0.2324	0.2754	0.2799	0.2324	0.2754	0.2799	0.2127	0.2765	0.2323	0.2127	0.2765	0.2323
29	wells_dist	0.0758	0.0587	0.0586	0.0758	0.0587	0.0586	0.0757	0.0606	0.0613	0.0757	0.0606	0.0613
30	wells	0.0817	0.0697	0.0680	0.0817	0.0697	0.0680	0.0812	0.0645	0.0673	0.0812	0.0645	0.0673

Table 14: This table provides per iteration training times for importance-weighted training for Gaussian q_ϕ optimized with our comprehensive step-search scheme. Please refer to Table 6 for lower-bound results.

Id	q_ϕ family Step-search scheme ∇_ϕ LI IWVI M_{training} IWVI M_{sampling} Independent Trial Model Name	Full-rank Gaussian Comprehensive step-search											
		Estimated without dropping the score-function term						Estimated with DReG					
		Used			Not Used			Used			Not Used		
		10			10			10			10		
		Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3
1	lsat	nan	nan	nan	nan	nan	nan	0.6082	0.6649	0.6574	0.6794	0.9469	0.6935
2	Mh	0.2637	0.2737	0.2745	0.2625	0.2658	0.2589	0.1373	0.1320	0.1278	0.1394	0.1295	0.1291
3	test_simplex	0.0137	0.0130	0.0122	0.0134	0.0127	0.0134	0.0129	0.0095	0.0096	0.0128	0.0086	0.0092
4	endo3	0.0544	0.0560	0.0574	0.0556	0.0561	0.0580	0.0372	0.0264	0.0264	0.0374	0.0262	0.0283
5	gp_predict	nan	1.0351	1.0520	1.0954	1.0511	1.0693	0.9513	0.8739	0.9259	0.9786	0.9526	nan
6	Mth	0.2582	0.2711	0.2728	0.2607	0.2811	0.2593	0.1007	0.1323	0.1152	0.1336	0.1679	0.1089
7	oxford	0.0933	0.0876	0.0928	0.1013	0.0977	0.0979	0.0543	0.0440	0.0428	0.0598	0.0485	0.0510
8	cjs_mnl	0.0199	0.0209	0.0208	0.0208	0.0207	0.0207	0.0196	0.0156	0.0153	0.0202	0.0157	0.0157
9	hepatitis	0.0759	0.0719	0.0722	0.0787	0.0760	0.0760	0.0458	0.0427	0.0354	0.0455	0.0375	0.0374
10	normal_multi	0.1689	0.1717	0.1734	0.1699	0.1686	0.1707	0.1636	0.1412	0.1310	0.1628	0.1402	0.1419
11	hiv_chr	0.0557	0.0554	0.0546	0.0561	0.0557	0.0554	0.0275	0.0301	0.0302	0.0362	0.0303	0.0300
12	electric_1c_chr	0.0358	0.0358	0.0363	0.0361	0.0369	0.0366	0.0289	0.0230	0.0230	0.0289	0.0240	0.0240
13	electric_1a_chr	0.0331	0.0331	0.0332	0.0333	0.0332	0.0335	0.0258	0.0230	0.0204	0.0273	0.0222	0.0223
14	electric_chr	0.0285	0.0279	0.0300	0.0288	0.0297	0.0299	0.0228	0.0187	0.0193	0.0228	0.0194	0.0191
15	radon_vary_si_chr	0.0564	0.0568	0.0570	0.0585	0.0595	0.0575	0.0394	0.0347	0.0325	0.0392	0.0321	0.0321
16	lda	0.0411	0.0427	0.0410	0.0416	0.0419	0.0418	0.0411	0.0428	0.0417	0.0413	0.0333	0.0349
17	radon_redundant_chr	0.0276	0.0275	0.0273	0.0284	0.0280	0.0277	0.0237	0.0190	0.0188	0.0239	0.0188	0.0191
18	naive_bayes	0.0929	0.0876	0.0881	0.0878	0.0901	0.0889	0.0878	0.0795	0.0793	0.0883	0.0704	0.0667
19	mesquite_volume	0.0127	0.0128	0.0128	0.0132	0.0133	0.0133	0.0128	0.0097	0.0098	0.0128	0.0099	0.0096
20	cjs_t_t	0.0948	0.0913	0.0913	0.0949	0.0899	0.0889	0.0875	0.0764	0.0767	0.0889	0.0798	0.0725
21	irt_multilevel	1.0576	0.8762	0.9683	1.3115	0.9599	1.0815	0.9164	0.7620	0.8797	0.9028	0.7732	0.8005
22	irt	0.9248	1.0201	0.9852	1.0918	0.8881	0.9860	0.9761	0.5699	0.7827	0.9187	0.7041	0.7859
23	congress	0.0188	0.0190	0.0190	0.0199	0.0194	0.0201	0.0194	0.0130	0.0130	0.0191	0.0129	0.0130
24	dogs	0.0386	0.0362	0.0360	0.0373	0.0373	0.0372	0.0372	0.0295	0.0313	0.0368	0.0311	0.0311
25	Dynocc	0.1145	0.1155	0.1266	0.1150	0.1156	0.1137	0.1145	0.1104	0.1113	0.1181	0.1094	0.1001
26	multi_logit	0.0910	0.0901	0.0915	0.0920	0.0910	0.0911	0.0917	0.0796	0.0769	0.0916	0.0825	0.0782
27	electric_one_pred	0.0141	0.0149	0.0144	0.0138	0.0146	0.0149	0.0143	0.0100	0.0100	0.0140	0.0109	0.0108
28	election88	0.2622	0.2345	0.2664	0.2677	0.2740	0.2724	0.2268	0.2689	0.2686	0.2063	0.2702	0.2688
29	wells_dist	0.0675	0.0690	0.0699	0.0689	0.0705	0.0688	0.0692	0.0528	0.0528	0.0681	0.0554	0.0549
30	wells	0.0749	0.0744	0.0741	0.0753	0.0743	0.0767	0.0750	0.0632	0.0624	0.0747	0.0590	0.0613

Table 15: This table provides per iterations training times for real-NVP normalizing flows optimized with our comprehensive step-search scheme with additional results from using IW-sampling. Please refer to Table 7 for lower-bound results.

Id	Model Name	Real NVP flows											
		Comprehensive step-search						Estimated with STL					
q_ϕ family	Step-search scheme	Estimated without dropping the score-function term						Estimated with STL					
∇_ϕ	LI	-full gradient						Not Used					
IWVI M_{training}	IWVI M_{sampling}	1			10			1			10		
Independent Trial	Model Name	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3
1	lsat	1.1155	1.4013	0.8866	1.1155	1.4013	0.8866	0.8995	1.2909	1.3146	0.8995	1.2909	1.3146
2	Mh	0.4176	0.3657	0.3984	0.4176	0.3657	0.3984	0.3917	0.5270	0.5304	0.3917	0.5270	0.5304
3	test_simplex	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan
4	endo3	0.2509	0.2287	0.2311	0.2509	0.2287	0.2311	0.2562	0.2643	0.2549	0.2562	0.2643	0.2549
5	gp_predict	1.3029	1.0646	1.1239	1.3029	1.0646	1.1239	1.1514	1.0246	1.3611	1.1514	1.0246	1.3611
6	Mth	0.4158	0.3843	0.3718	0.4158	0.3843	0.3718	0.4255	0.5200	0.5311	0.4255	0.5200	0.5311
7	oxford	0.2828	0.2770	0.2678	0.2828	0.2770	0.2678	0.3053	0.2851	0.2996	0.3053	0.2851	0.2996
8	cjs_mnl	0.1424	0.1426	0.1459	0.1424	0.1426	0.1459	0.1936	0.1972	0.2079	0.1936	0.1972	0.2079
9	hepatitis	0.2471	0.2461	0.2467	0.2471	0.2461	0.2467	0.2720	0.2732	0.2724	0.2720	0.2732	0.2724
10	normal_multi	0.3088	0.3743	0.3030	0.3088	0.3743	0.3030	0.3247	0.3106	0.3868	0.3247	0.3106	0.3868
11	hiv_chr	0.2298	0.2091	0.2803	0.2298	0.2091	0.2803	0.2528	0.3103	0.3063	0.2528	0.3103	0.3063
12	electric_1c_chr	0.1899	0.2002	0.2004	0.1899	0.2002	0.2004	0.2110	0.1990	0.1888	0.2110	0.1990	0.1888
13	electric_1a_chr	0.1808	0.1958	0.1964	0.1808	0.1958	0.1964	0.2173	0.2198	0.2175	0.2173	0.2198	0.2175
14	electric_chr	0.1869	0.1794	0.1789	0.1869	0.1794	0.1789	0.2048	0.2053	0.2054	0.2048	0.2053	0.2054
15	radon_vary_si_chr	0.2396	0.2797	0.1970	0.2396	0.2797	0.1970	0.2552	0.2473	0.2442	0.2552	0.2473	0.2442
16	lda	nan	0.1483	nan	nan	0.1483	nan	nan	nan	nan	nan	nan	nan
17	radon_redundant_chr	0.1739	0.1640	0.1721	0.1739	0.1640	0.1721	0.1898	0.1959	0.1988	0.1898	0.1959	0.1988
18	naive_bayes	0.2366	0.2179	0.2147	0.2366	0.2179	0.2147	0.2365	0.2295	0.2384	0.2365	0.2295	0.2384
19	mesquite_volume	0.1289	0.1246	0.1249	0.1289	0.1246	0.1249	0.1508	0.1265	0.1484	0.1508	0.1265	0.1484
20	cjs_t_t	0.2017	0.2044	0.2041	0.2017	0.2044	0.2041	0.2159	0.2679	0.2090	0.2159	0.2679	0.2090
21	irt_multilevel	1.0242	1.1134	1.2535	1.0242	1.1134	1.2535	0.9318	1.1821	1.2016	0.9318	1.1821	1.2016
22	irt	1.0350	1.3052	1.1808	1.0350	1.3052	1.1808	1.1201	0.9608	1.1653	1.1201	0.9608	1.1653
23	congress	0.1310	0.1355	0.1354	0.1310	0.1355	0.1354	0.1832	0.1877	0.1922	0.1832	0.1877	0.1922
24	dogs	0.1495	0.1989	0.1571	0.1495	0.1989	0.1571	0.1617	0.1622	0.1631	0.1617	0.1622	0.1631
25	Dynocc	0.2708	0.2380	0.2273	0.2708	0.2380	0.2273	0.2886	0.2308	0.2843	0.2886	0.2308	0.2843
26	multi_logit	0.2261	0.2043	0.2153	0.2261	0.2043	0.2153	0.2235	0.2278	0.2367	0.2235	0.2278	0.2367
27	electric_one_pred	0.1318	0.1232	0.1317	0.1318	0.1232	0.1317	0.1776	0.1792	0.2418	0.1776	0.1792	0.2418
28	election88	0.3636	0.3676	0.3965	0.3636	0.3676	0.3965	0.3134	0.3739	0.4694	0.3134	0.3739	0.4694
29	wells_dist	0.1663	0.2459	0.1756	0.1663	0.2459	0.1756	0.2180	0.2328	0.2324	0.2180	0.2328	0.2324
30	wells	0.1934	0.1830	0.1756	0.1934	0.1830	0.1756	0.2571	0.2318	0.1722	0.2571	0.2318	0.1722

Table 16: This table provides per iteration training times for importance weighted training for real-NVP normalizing flows optimized with our comprehensive step-search scheme with additional results from using regular IW-ELBO gradient. Please refer to [Table 8](#) for lower-bound results.

Id	q_ϕ family Step-search scheme ∇_ϕ	Real NVP flows					
		Comprehensive step-search			Estimated with DReG		
		Estimated w/o dropping score-function term			Estimated with DReG		
	LI	Not Used			Not Used		
	IWVI M_{training}	10			10		
	IWVI M_{sampling}	10			10		
	Independent Trial	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3
	Model Name						
1	lsat	1.3123	1.3801	0.8872	1.3382	1.1976	1.2966
2	Mh	0.4034	0.3471	0.3457	0.4056	0.5139	0.4923
3	test_simplex	nan	nan	nan	nan	nan	nan
4	endo3	0.2403	0.2181	0.2214	0.2415	0.2480	0.2020
5	gp_predict	1.2093	1.3739	1.1092	1.0965	1.1590	1.2996
6	Mth	0.4022	0.3624	0.3600	0.3844	0.5129	0.4950
7	oxford	0.2711	0.2679	0.2685	0.2874	0.2765	0.2786
8	cjs_mnl	0.1344	0.1333	0.1365	0.1682	0.1452	0.1803
9	hepatitis	0.2365	0.2357	0.2366	0.2652	0.2565	0.2503
10	normal_multi	0.2988	0.3720	0.2505	0.3044	0.3897	0.2691
11	hiv_chr	0.2192	0.1919	0.2701	0.2368	0.2876	0.2792
12	electric_1c_chr	0.1797	0.1884	0.1895	0.1982	0.2019	0.1882
13	electric_1a_chr	0.1736	0.1854	0.1851	0.2022	0.1953	0.1974
14	electric_chr	0.1771	0.1756	0.1707	0.1911	0.2218	0.1918
15	radon_vary_si_chr	0.2386	0.2184	0.2069	0.2386	0.2347	0.2722
16	lda	0.1566	0.1510	0.1477	0.2008	nan	0.2252
17	radon_redundant_chr	0.1726	0.1641	0.1545	0.1913	0.1575	0.1830
18	naive_bayes	0.2059	0.2079	0.2053	0.2205	0.2174	0.2012
19	mesquite_volume	0.1174	0.1223	0.1155	0.1608	0.1679	0.1167
20	cjs_t_t	0.1875	0.1970	0.1942	0.2004	0.2206	0.1759
21	irt_multilevel	1.0148	1.1641	1.0829	1.0970	1.1833	1.1628
22	irt	1.1033	0.8217	1.1170	1.0006	0.9708	1.1640
23	congress	0.1214	0.1284	0.1267	0.1623	0.1694	0.1675
24	dogs	0.1407	0.1797	0.1925	0.1487	0.1559	0.1500
25	Dynocc	0.2327	0.2272	0.2273	0.2690	0.2357	0.2853
26	multi_logit	0.2138	0.1946	0.2068	0.2201	0.2298	0.2244
27	electric_one_pred	0.1209	0.1150	0.1201	0.1585	0.1612	0.1601
28	election88	0.3934	0.3862	0.3583	0.3379	0.4366	0.3613
29	wells_dist	0.1652	0.2018	0.2176	0.1758	0.1630	0.2141
30	wells	0.2027	0.1720	0.1730	0.2212	0.2187	0.1587

Table 17: This table presents the per iteration training time for additional Diagonal Gaussian experiments. Please refer to [Figure 11](#) and [appendix B](#) for more details.

Id	Model Name	Diagonal Gaussian								
		Comprehensive step-search			Estimated with STL			Closed form entropy		
	q_ϕ family									
	Step-search scheme									
	∇_ϕ									
	LI	Not Used			Not Used					
	IWVI M_{training}	1			1					
	IWVI M_{sampling}	1			1			10		
	Independent Trial	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3	Trial 1	Trial 2	Trial 3
1	lsat	0.1602	0.1479	0.1616	0.7932	0.5420	0.5403	0.7932	0.5420	0.5403
2	Mh	0.0754	0.0682	0.0753	0.1278	0.1227	0.1240	0.1278	0.1227	0.1240
3	test_simplex	0.0138	0.0147	0.0150	0.0156	0.0147	0.0154	0.0156	0.0147	0.0154
4	endo3	0.0274	0.0274	0.0288	0.0350	0.0347	0.0352	0.0350	0.0347	0.0352
5	gp_predict	0.8618	0.8190	1.0537	1.1967	1.2193	1.1846	1.1967	1.2193	1.1846
6	Mth	0.0719	0.0719	0.0702	0.1196	0.1231	0.1209	0.1196	0.1231	0.1209
7	oxford	0.0343	0.0339	0.0341	0.0471	0.0458	0.0485	0.0471	0.0458	0.0485
8	cjs_mnl	0.0178	0.0208	0.0193	0.0211	0.0207	0.0211	0.0211	0.0207	0.0211
9	hepatitis	0.0251	0.0279	0.0249	0.0388	0.0393	0.0386	0.0388	0.0393	0.0386
10	normal_multi	0.1237	0.1247	0.1244	0.1245	0.1481	0.1476	0.1245	0.1481	0.1476
11	hiv_chr	0.0261	0.0246	0.0261	0.0320	0.0332	0.0321	0.0320	0.0332	0.0321
12	electric_1c_chr	0.0250	0.0240	0.0245	0.0288	0.0274	0.0273	0.0288	0.0274	0.0273
13	electric_1a_chr	0.0230	0.0249	0.0216	0.0269	0.0264	0.0264	0.0269	0.0264	0.0264
14	electric_chr	0.0224	0.0210	0.0199	0.0242	0.0241	0.0241	0.0242	0.0241	0.0241
15	radon_vary_si_chr	0.0252	0.0285	0.0303	0.0352	0.0358	0.0351	0.0352	0.0358	0.0351
16	lda	0.0386	0.0374	0.0384	0.0395	0.0416	0.0414	0.0395	0.0416	0.0414
17	radon_redundant_chr	0.0200	0.0215	0.0201	0.0234	0.0239	0.0240	0.0234	0.0239	0.0240
18	naive_bayes	0.0736	0.0744	0.0658	0.0870	0.0859	0.0859	0.0870	0.0859	0.0859
19	mesquite_volume	0.0143	0.0140	0.0142	0.0145	0.0167	0.0145	0.0145	0.0167	0.0145
20	cjs_t_t	0.0860	0.0680	0.0831	0.0847	0.0756	0.0855	0.0847	0.0756	0.0855
21	irt_multilevel	0.6101	0.6449	0.6103	0.9602	0.9485	0.9637	0.9602	0.9485	0.9637
22	irt	0.6141	0.6213	0.5945	0.9598	0.7211	0.9360	0.9598	0.7211	0.9360
23	congress	0.0184	0.0181	0.0174	0.0185	0.0205	0.0185	0.0185	0.0205	0.0185
24	dogs	0.0347	0.0340	0.0358	0.0347	0.0337	0.0347	0.0347	0.0337	0.0347
25	Dynocc	0.1117	0.0915	0.0903	0.1054	0.1175	0.1164	0.1054	0.1175	0.1164
26	multi_logit	0.0776	0.0807	0.0719	0.0800	0.0851	0.0853	0.0800	0.0851	0.0853
27	electric_one_pred	0.0144	0.0164	0.0144	0.0154	0.0152	0.0154	0.0154	0.0152	0.0154
28	election88	0.2186	0.2183	0.2189	0.2808	0.2346	0.2838	0.2808	0.2346	0.2838
29	wells_dist	0.0507	0.0569	0.0538	0.0587	0.0592	0.0587	0.0587	0.0592	0.0587
30	wells	0.0652	0.0602	0.0724	0.0671	0.0685	0.0667	0.0671	0.0685	0.0667