Bayesian Non-linear Regression

Václav Šmídl

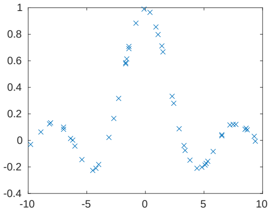
May 5, 2020

Limit of linear models – basis functions

Fit by a linear combination of basis functions:

$$y_i \quad = a\phi_1(x_i) \quad + b\phi_2(x_i) \quad + e_i$$

What should be the basis function?



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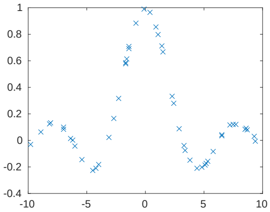
where ϕ_j are non-linear functions with parameters ψ_k.

Estimating new set of parameters $\theta = [a, b, \psi_1, \psi_2]$

$$\frac{d(y_i - a\phi_1(\psi_1, x_i) + b\phi_2(\psi_2, x_i))^2}{d\theta} = 0.$$

$$\hat{\theta} = ?$$



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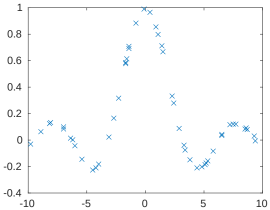

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$$\phi_j(x_i, W, b) = \tanh(Wx_i + b),$$
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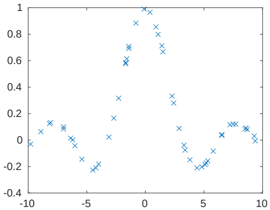

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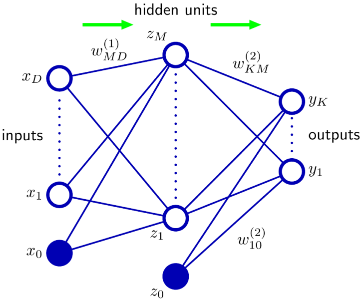
Nested functions

$$\tanh(W_1 \tanh(W_2 x_i + b_2) + b_1),$$

Neural networks

Feed forward NN:

$$z_1 = \sigma_1 (W_1 x + b_1),$$
$$z_2 = \sigma_2 (W_2 z_1 + b_2), \ldots$$
$$y = \sigma_2 (w_m z_m + b_m) + e$$



with vector-valued
– **activation** functions $\sigma_j()$,
– **weights** w_j
– **biases** b_i.

For Gaussian noise, maximum log-likelihood is

$$\hat{\theta} = \arg\min \mathcal{L}(x, y, \theta), \quad \mathcal{L} = \boldsymbol{e}^T \boldsymbol{e} = \sum_{i=1}^{n} (y_i - \sigma_1 (w_1 \sigma_2 (\cdots) + b_1))^2 .$$

MSE (mean square error) loss function with unknowns
$\theta = [w_1, b_1, w_2, b_2, \ldots,]$.

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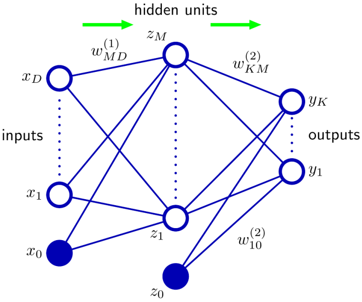

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MSE (mean square error) loss function with unknowns $\theta = [w_1, b_1, w_2, b_2, \ldots,]$. Gradient descent method

$$\hat{\theta}^{(\tau+1)} = \hat{\theta}^{(\tau)} - \eta \nabla \mathcal{L}(\hat{\theta}^{(\tau)}),$$

where η is the (small) learning rate.

Example

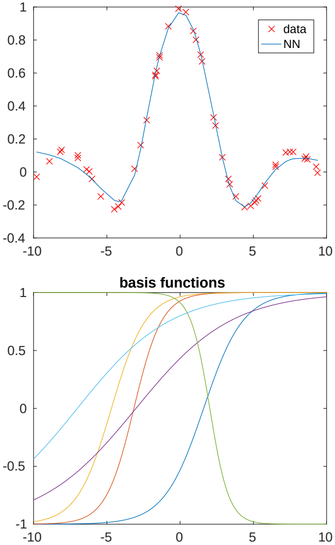
Trivial NN with one hidden layer:

$$y_i = \sum_{i=1}^{6} w_{2,i} \tanh(w_{1,j} x_i + b_{1,j}) + b_2,$$

tanh activation function on hidden layer and linear activation function on output.
Training by GD:

1. random initialization,
2. 50000 steps,
3. rate $\eta = 0.001$,

Main issue: reliability, slow convergence,...

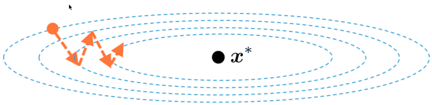


Faster gradient descent

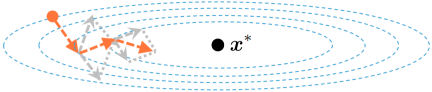
In general, gradient descent requires $O(1/\epsilon)$ steps

$$\frac{2L(\mathcal{L}\{(\hat{\theta}^{(0)}) - \mathcal{L}\{(\theta^*))}{\epsilon} \leq \tau_{max}$$

where L is the Lipschitz constant of $\mathcal{L}$, for **convex** function.



gradient descent



heavy-ball method

Heavy-ball (momentum): accumulate velocity

$$\hat{\theta}^{(\tau+1)} = \hat{\theta}^{(\tau)} - \eta \nabla L(\hat{\theta}^{(\tau)}) + \beta(\hat{\theta}^{(\tau)} - \hat{\theta}^{(\tau-1)})$$

has theoretical asymptotic number of steps $O(1/\sqrt{\epsilon})$.

- Nesterov: theoretically the fastest first-order method. Tuning: η, β (via L?)

Second-order: Newton method

Optimize:

$$\hat{\theta} = \arg\min_{\theta} \mathcal{L}(\theta)$$

using Taylor expansion

$$\mathcal{L}(\theta^{(\tau)} + \boldsymbol{h}) \approx \mathcal{L}(\theta^{(\tau)}) + \nabla \mathcal{L}(\theta^{(\tau)})\boldsymbol{h} + \frac{1}{2}\boldsymbol{h}^T H_{\mathcal{L}}(\theta_k)\boldsymbol{h}$$

where $H_{\mathcal{L}}(\theta) = \nabla^2 \mathcal{L}(\theta)$.

We wish that $\theta^{(\tau+1)} = \theta^{(\tau)} + \boldsymbol{h}$ is an optimum, i.e. $\nabla_{\boldsymbol{h}} \mathcal{L}(\theta_k + \boldsymbol{h}) \equiv 0$:

$$\nabla \mathcal{L}(\theta^{(\tau)}) + H_{\mathcal{L}}(\theta^{(\tau)})\boldsymbol{h} = 0 \quad \Leftrightarrow \quad \boldsymbol{h} = -\left(H_{\mathcal{L}}(\theta^{(\tau)})\right)^{-1} \nabla \mathcal{L}(\theta^{(\tau)})$$

yielding

$$\theta^{(\tau+1)} = \theta^{(\tau)} - H_{\mathcal{L}}(\theta^{(\tau)})^{-1} \nabla \mathcal{L}(\theta^{(\tau)}).$$

with theoretical asymptotic number of steps $O(\log(\log \epsilon))$. (Expensive steps!)

Approximation of the Hessian: **LBFGS**.

Stochastic Gradient Descent

Original loss function

$$\mathcal{L}(y,x,\theta) = \sum_{i=1}^{n} \left(y_i - \sigma_1\left(w_1\sigma_2\left(\cdots\right) + b_1\right)\right)^2 .$$

is replaced by:

$$\tilde{\mathcal{L}}(y,x,\theta) = \sum_{i\in\mathcal{I}} \left(y_i - \sigma_1\left(w_1\sigma_2\left(\cdots\right) + b_1\right)\right)^2 .$$

where $\mathcal{I} \subset \{1,\ldots,n\}, |\mathcal{I}| \ll n$. For random samples of indeces $j = 1,\ldots m$,

$$\nabla_\theta \mathcal{L}(y,x,\theta) = \mathrm{E}\left(\nabla\tilde{\mathcal{L}}(y,x,\theta)\right)$$

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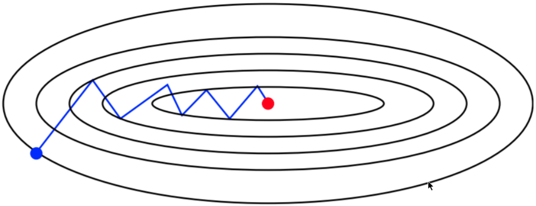
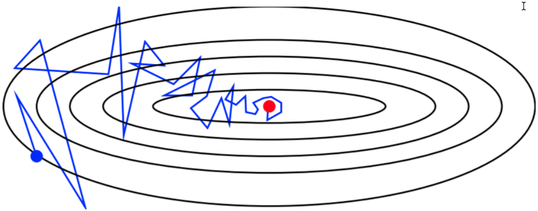
Stochastic Gradient Descent

Deterministic gradient:



Stochastic gradient: will converge only if $\eta_\tau \to 0$.

For constant η_τ it "walks" around optima.



Adaptive Learning Rate SGD

AdaGrad (Duchi, 2011) method uses estimate of the Hessian

$$H_{\mathcal{L}}(\hat{\theta}) \approx \mathrm{diag}(\sqrt{\boldsymbol{r}_{\tau+1}}),$$
$$\boldsymbol{r}_{\tau+1} = \boldsymbol{r}_{\tau} + \left[\nabla \tilde{\mathcal{L}}(\hat{\theta}^{(\tau)})\right].^{2}$$

accumulates all values from the beginning (infinite window) .

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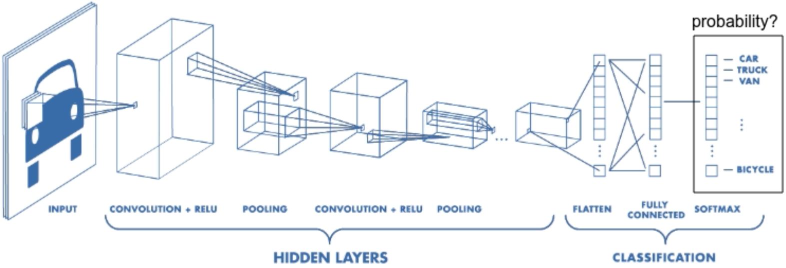
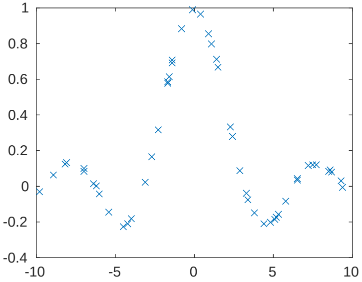
Controversy: adaptation can help but can also harm convergence

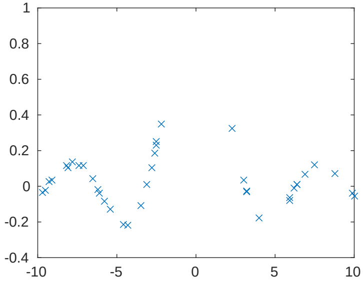
Deep Learning



- Large networks with many layers
- Special layers that allow to compute gradients
- Training by a first-order methods
- Excellent at supervised tasks (regression)

Can we trust the result?





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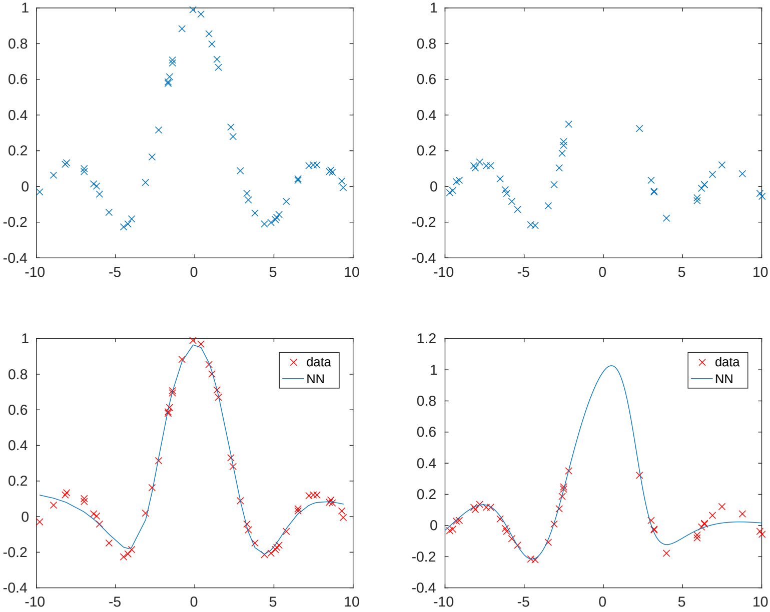
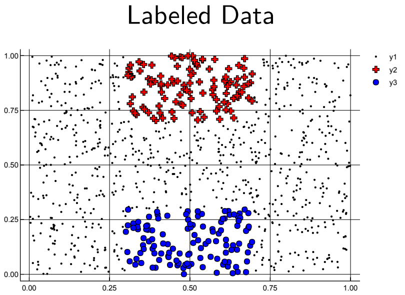
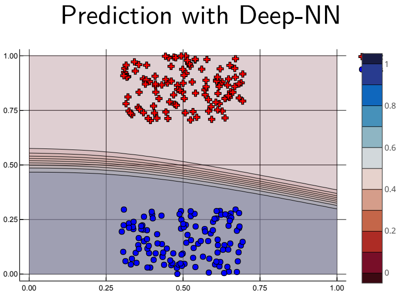


False confidence in classification





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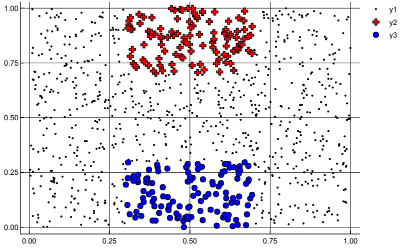
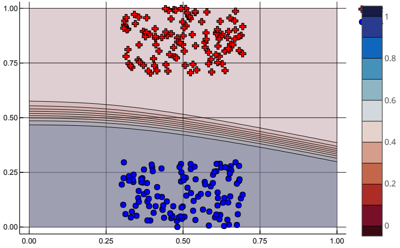
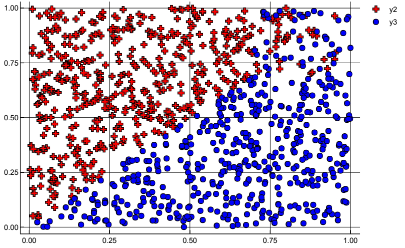


Prediction with Deep-NN



True labels



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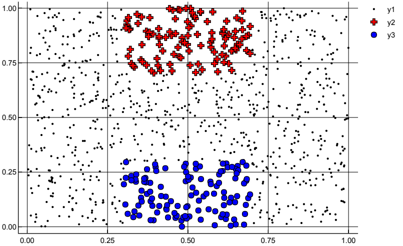

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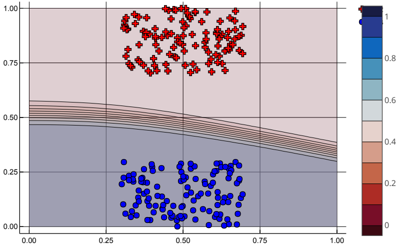

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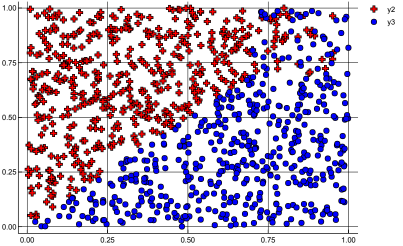
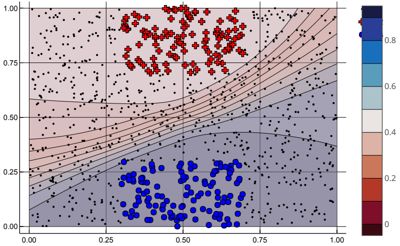


$\int p(y|\theta, x)p(\theta)d\theta$ from 500 HMC



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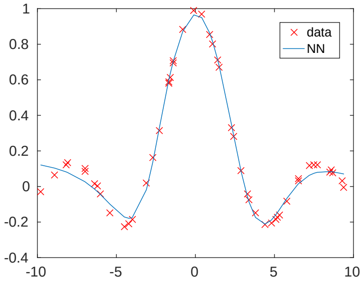
Langevin Dynamics (Welling, Teh, 2011):

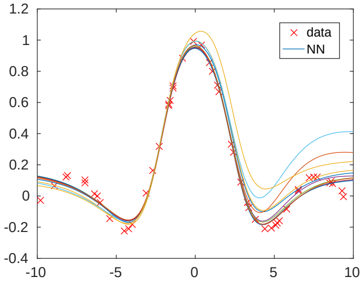
$$\hat{\theta}^{(\tau+1)} = \hat{\theta}^{(\tau)} - \eta \nabla \tilde{L}(\hat{\theta}^{(\tau)}) + e_t, \quad e_t \sim \mathcal{N}(0, \epsilon),$$

where ϵ and η needs to be carefully balanced. (Asymptotic proof of acceptance rate=1).

Laplace



max+0.1std



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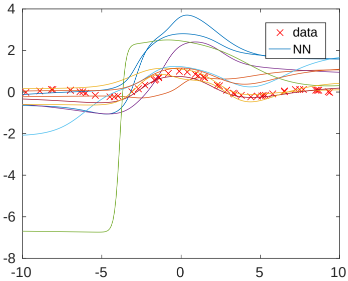
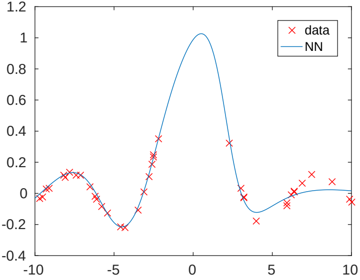


Laplace II



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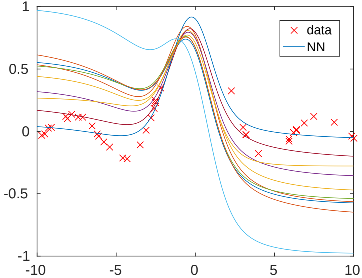

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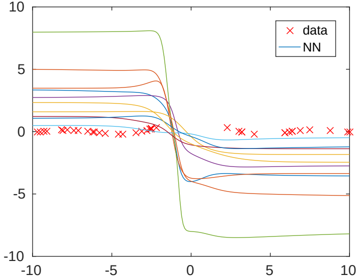
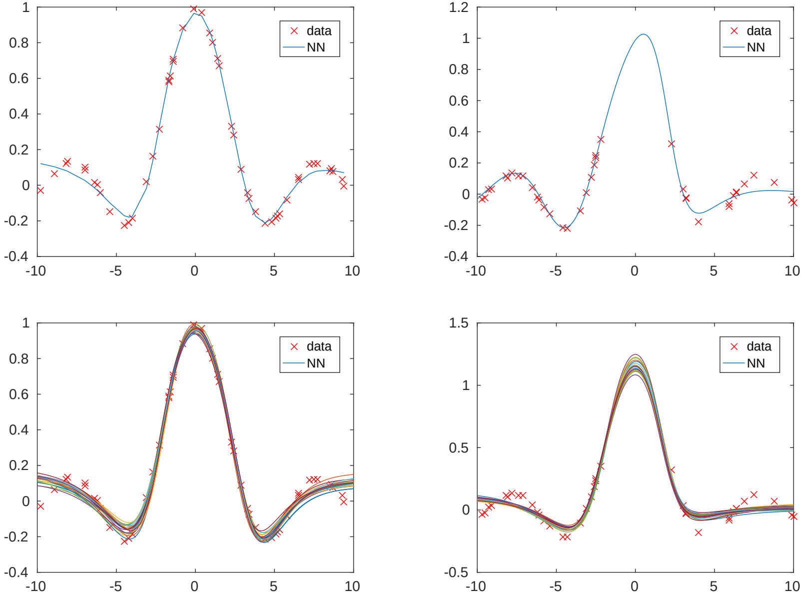


Langevin MCMC (tweaked)



Uncertainty in the number of basis functions

- Knowing that the "true" value of the basis functions is 6 is very strong information.
- How many basis functions for an arbitrary function? Universal approximation property of NN. Infinity.
- Limit of 2 layer NN is the Gaussian process (Neal, 1994):

$$y(x) \sim GP(0, K(\theta, x, x'))),$$

  where $K(x, x')$ is a covariance function of all possible x, x' pairs, and θ is a hyperparameter.
- For a chosen vector of $\boldsymbol{x}$ has Gaussian distribution with

$$y \sim \mathcal{N}(0, K(\theta, \boldsymbol{x}, \boldsymbol{x}'))).$$

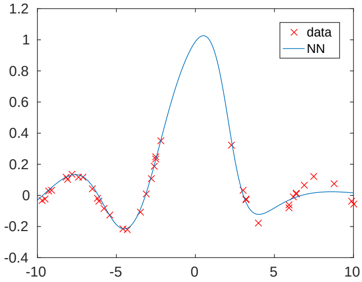
- Joint process of testing new data $\overline{x}$ using training data x (Rasmussen, 2006)

$$\begin{bmatrix} y(x) \\ \overline{y}(\overline{x}) \end{bmatrix} \sim GP\left(0, \begin{bmatrix} K(x, x') & K(x, \overline{x}') \\ K(\overline{x}, x') & K(\overline{x}, \overline{x}') \end{bmatrix}\right),$$

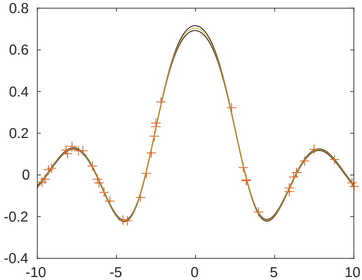
  and predictive points are marginal

$$\overline{y}(\overline{x}) \sim \mathcal{N}(K(\overline{x}, x')K(x, x')^{-1}y(x), K(\overline{x}, \overline{x}') - K(\overline{x}, x')K(x, x')^{-1}K(x, \overline{x}'))$$

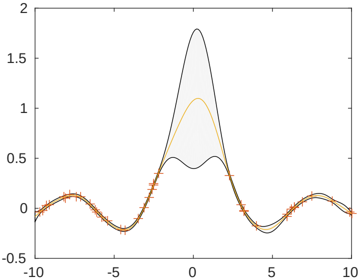
Gaussian process and its hyperparameters



GP: empirical Bayes kernel



GP: inflated kernel



Dropout MC

Standard Network Model:

$$
\begin{aligned}
z_i &= \sigma_i\left(W_i x + b_i\right), \quad i = 1 : m-1, \\
y &= \sigma_2\left(w_m z_m + b_m\right),
\end{aligned}
$$

Dropout Network Model:

$$
\begin{aligned}
z_i &= \sigma_i\left(W_i\left(\xi_i \circ x\right) + b_1\right), \\
y &= \sigma_2\left(w_m(\xi_m \circ z_m) + b_m\right)
\end{aligned}
$$

where ξ_i are vectors of zeros and ones sampled from Bernouli distribution.

Works also for Gaussian distribution, can be explained by Variational Inference.

- Dropout is an approximation of GP (Gal, Ghahramani, 2016),
- Deep Neural Networks as Gaussian Processes (Lee, et. al. 2018).

SGD is Approximate Bayesian Inference

SDG is a discretization of approximation of random walk model

$$\nabla \tilde{\mathcal{L}}(\theta) \approx \nabla \mathcal{L}(\theta) + \frac{1}{\sqrt{S}}\Delta, \qquad \Delta \sim \mathcal{N}(0, C(\theta))$$

If the loss function can be approximated by quadratic function

$$\mathcal{L}(\theta) = \frac{1}{2}\theta^\top A\theta,$$

then posterior factor $q(\theta) = \mathcal{N}(\hat{\theta}, \Sigma)$ satisfies:

$$\Sigma A + A\Sigma = \frac{\eta}{S} C(\theta).$$

Minimizing KL to $p(\theta)$ yields (Mandt, Hoffman, Blei, 2017):

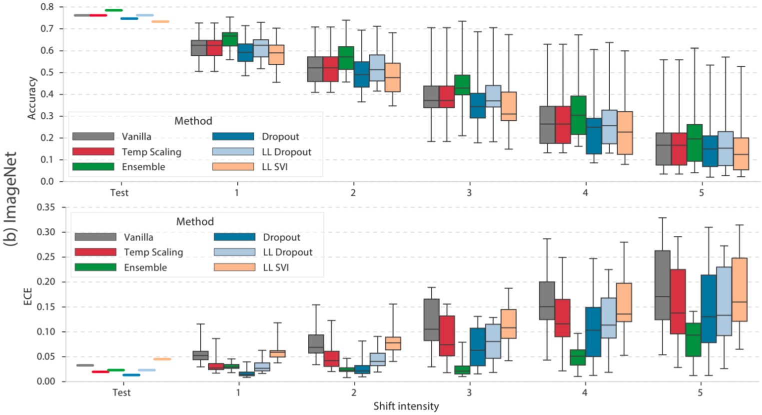
$$\eta^* = \frac{2S}{N}\frac{\dim(\theta)}{\mathrm{tr}(C)}, \text{ or } \qquad H^* = \frac{2S}{N} C^{-1}, \text{ (matrix learning rate)}$$

Can be used to tune learning rate using

$$C_\tau = (1 - \kappa_\tau)C_{\tau-1} + \kappa_\tau \mathrm{cov}(\nabla\tilde{\mathcal{L}}).$$

Sad story: Large scale comparison

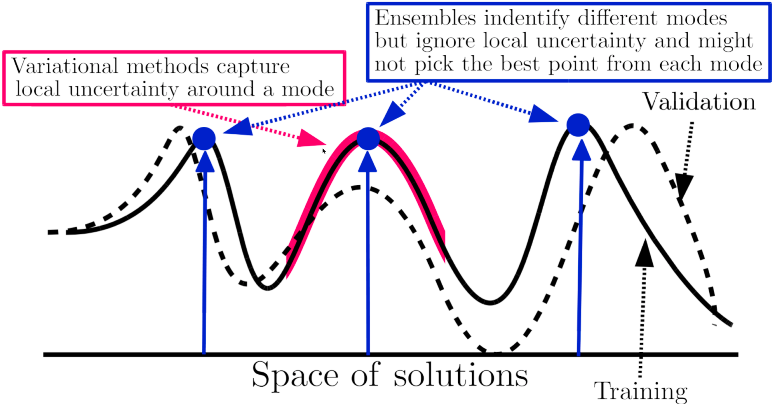
Various methods were compared in (Ovadia, et. al 2019):



The winner is **ensemble**: parallel run of NN from different starts.

Landscape of Deep networks

Hypothesis (Fort et. al. 2019): The probability of weights in networks is multimodal:



Assignment:

- Create a 1d regression problem with missing data
- train neural network fro minimum loss
- try one of the Bayesian approaches
  - Laplace,
  - Dropout
  - Ensemble
  - Langevin
  - HMC...