Bayesian Non-linear Regression: Gradient Approach

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Recapitulation

Monte Carlo methods

- MCMC
- HMC

Properties:

- convergence to the true solution
- simplicity
- correlation

Least Squares

Linear regression:

$$\mathbf{y} = X\theta + \mathbf{e},$$

Minimize

$$\sum_i e_i^2 = \mathbf{e}^T\mathbf{e} = (\mathbf{y} - X\theta)^\top(\mathbf{y} - X\theta)$$

$$\frac{d}{d\theta}((\mathbf{y} - X\theta)^T(\mathbf{y} - X\theta)) = 0$$

$$\frac{d}{d\theta}(\mathbf{y}^T\mathbf{y} - \theta^T X^T\mathbf{y} - \mathbf{y}^T X\theta + \theta^T X^T X\theta) = 0$$

$$X^T X\theta = X^T\mathbf{y}$$

Analytical:

$$\hat{\theta} = (X^T X)^{-1} X^T\mathbf{y}.$$

For large θ, conjugate gradients.

Gradient Descent:

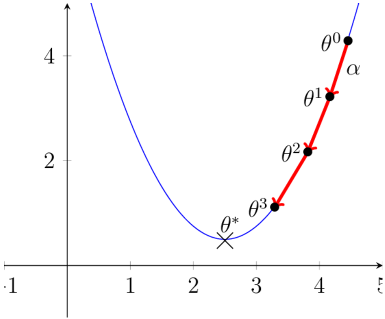
Gradient descent (GD, 1st order):

$$\hat{\theta} = \arg\min_{\theta \in \Theta} \mathcal{L}$$

$$\hat{\theta}_{k+1} = \hat{\theta}_k - \alpha \nabla_\theta \mathcal{L}$$

$$\hat{\theta}_{k+1} = \hat{\theta}_{k+1} - \alpha (X^T X \theta_k - X^T \mathbf{y})$$

Very many cheap (GPU) iterations.



Beyond Linear Regression

Linear regression can fit arbitrary combination of **known** basis functions:

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\begin{aligned}
y &= a + bx + cx^2 + dx^3 && = [1, x, x^2, x^3]\theta \\
y &= a \exp(cx) + b \exp(dx) && = [\exp(cx), \exp(dx)]\theta
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What if the exponent decay of bi-exponential is not known? Common in functional medical imaging.

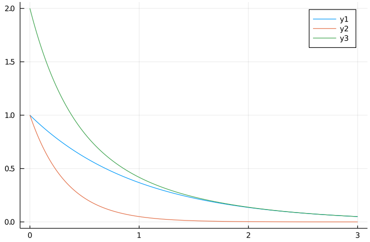
Include them in optimization, $\theta = [a, b, c, d]$, of least-squares

$$\hat{\theta} = \arg\min_{\theta} \sum_{i=1}^{n} (y_i - f(x))^2$$

$$f(x) = a\exp(cx_i) - b\exp(dx_i)$$

and run GD (or other optimization) .

- Run in Matlab cftoolbox.



Interpretation point of view

Without knowing it, the biologist used a neural network.

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Specifically Multi-layer perceptron (MLP), with 2-layers, and 2 hidden units.

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1. exp activation function:

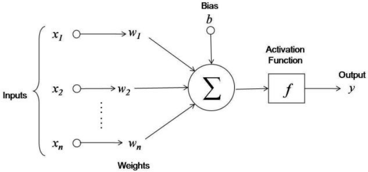
$$z_i = \exp(w_{1,i}x), i = 1, 2$$

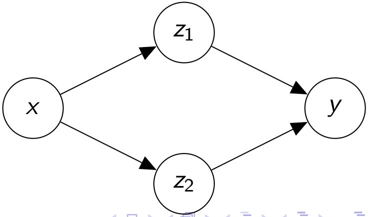
2. linear activation function:

$$y = \sum_{i=1}^{2} w_{2,i} z_i$$

MLP is a regression that learns basis functions from the data!

- known as "dense" layers now.



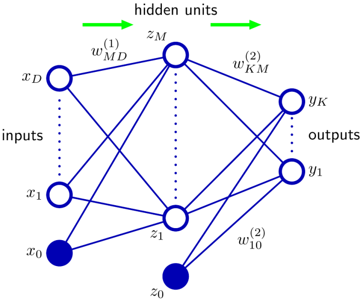


Neural networks

Feed forward NN:

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

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



For Gaussian noise, maximum log-likelihood is

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

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

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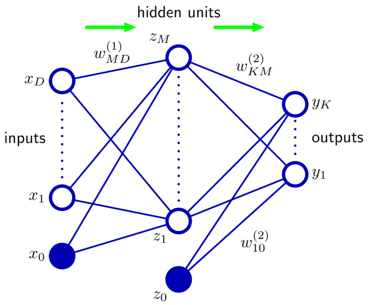

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MSE (mean square error) loss function with unknowns $\theta = [w_1, b_1, w_2, b_2, \ldots,]$. Gradient descent method

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

where η is the (small) learning rate.

Example

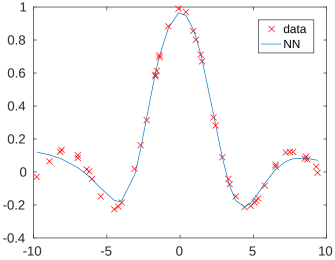
Trivial NN with one hidden layer:

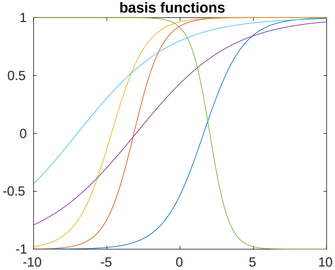
$$y_i = \sum_{i=1}^{6} w_{2,i} \tanh(w_{1,j} x_i + b_{1,j}) + b_2,$$

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,...



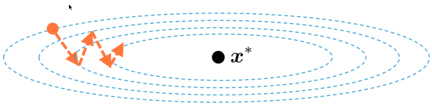


Faster gradient descent

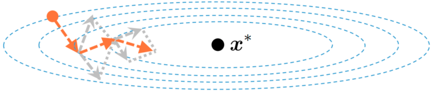
In general, gradient descent requires $O(1/\epsilon)$ steps

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

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**.

Example: Newton for OLS

Gradient descent (GD, 1st order):

$$\hat{\theta} = \arg\min_{\theta \in \Theta} \mathcal{L}$$

$$\hat{\theta}_{k+1} = \hat{\theta}_k - \alpha \nabla_\theta \mathcal{L}$$

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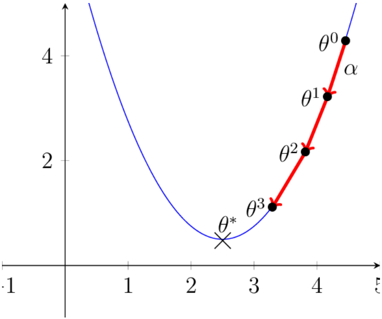
Very many cheap (GPU) iterations.



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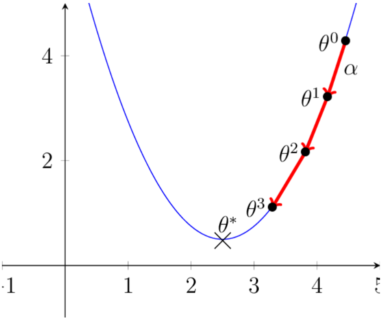
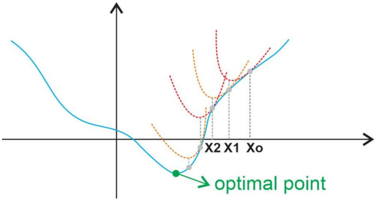


Newton's method (2nd order):

$$\hat{\theta}_{k+1} = \hat{\theta}_k - H_\theta^{-1} \nabla_\theta \mathcal{L}$$

$$\hat{\theta}_{k+1} = \hat{\theta}_k - (X^T X)^{-1}(X^T X \hat{\theta}_k - X^T \mathbf{y})$$

$$= (X^T X)^{-1}(X^T \mathbf{y})$$



One expensive iteration.
Infeasible in high dimensions

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 $j = 1, \ldots m$,

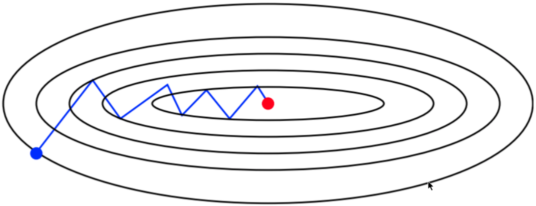
$$\nabla_\theta \mathcal{L}(y, x, \theta) = \mathrm{E}\left(\nabla \tilde{\mathcal{L}}(y, x, \theta)\right)$$

yielding

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

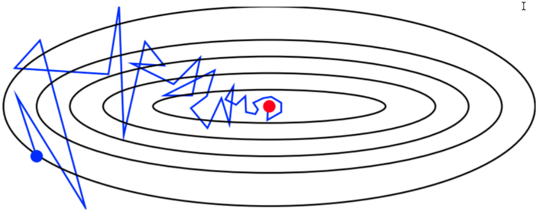
Stochastic Gradient Descent

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

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

accumulates all values from the beginning (infinite window) .

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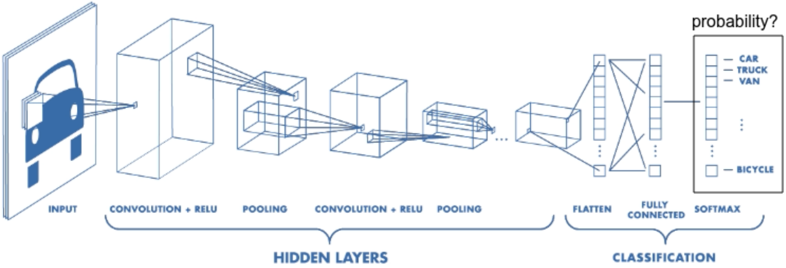
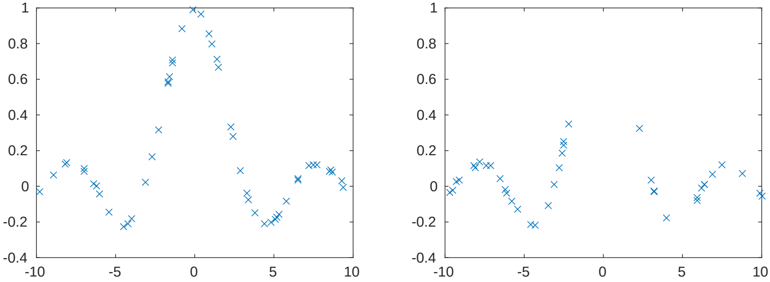
Controversy: adaptation can help but can also harm convergence

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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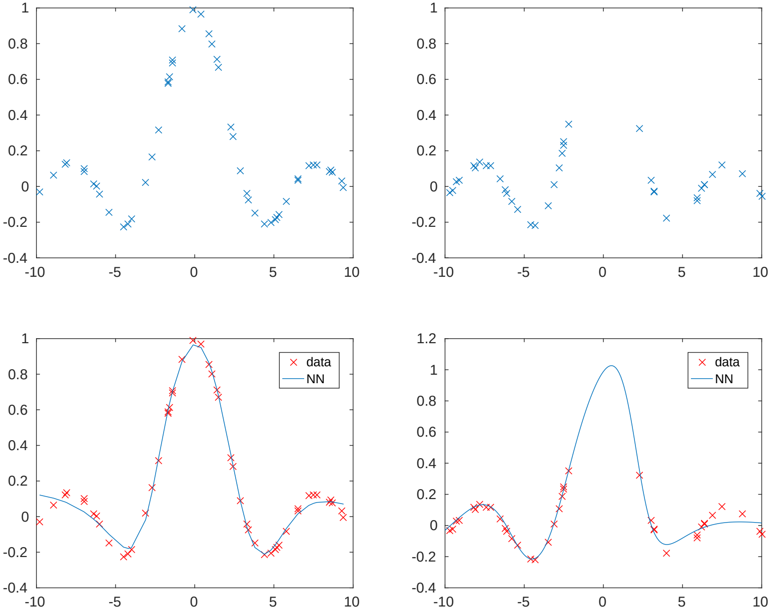

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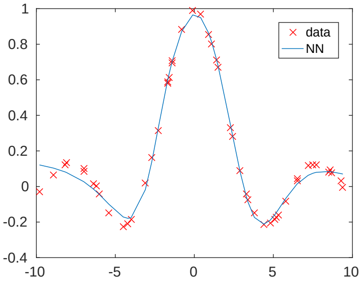

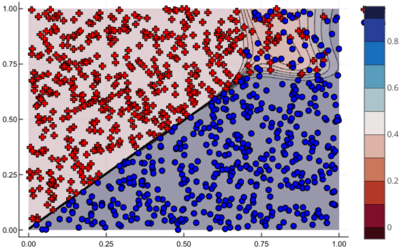

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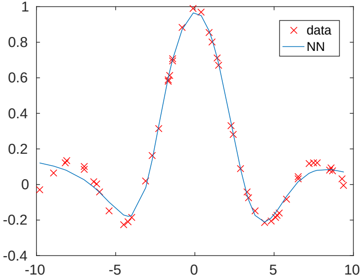

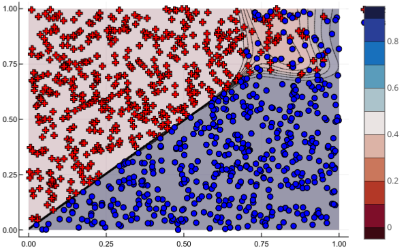

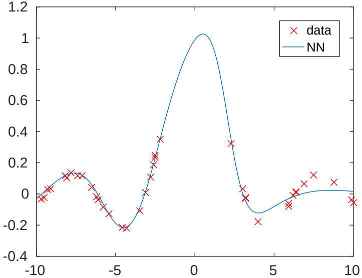

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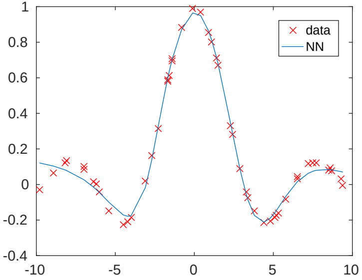

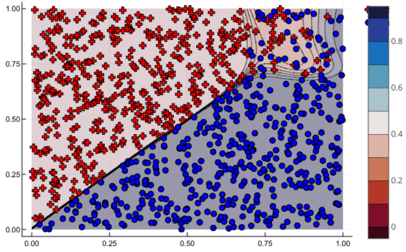

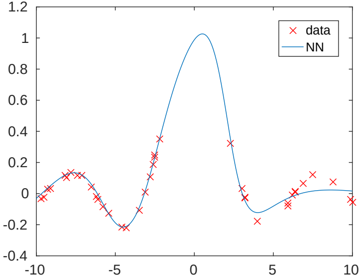

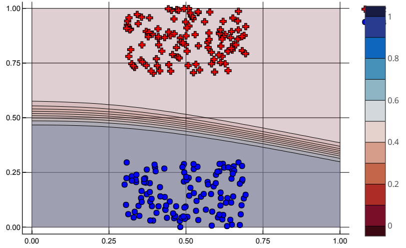

Two kinds of uncertainty

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Epistemic uncertainty:

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Epistemic uncertainty:

- lack of knowledge,
- systematic model insufficiency,
- can be reduced.
- handled by Bayesian approaches
  - neural network parameters have posterior distributions

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Replace parameter estimate $\hat{\theta}$ by $p(\theta)$. Harder than with linear models:

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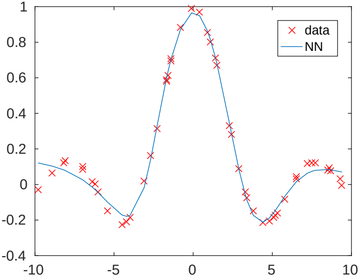
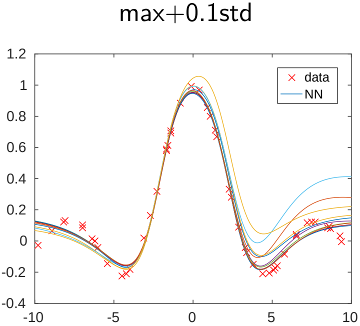
Langevin Dynamics (Welling, Teh, 2011):

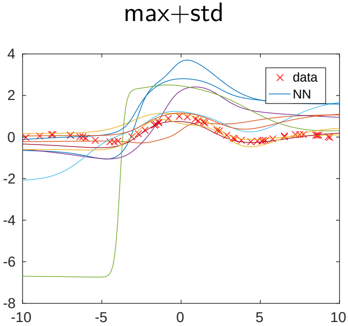
$$\hat{\theta}^{(\tau+1)} = \hat{\theta}^{(\tau)} - \eta\nabla\tilde{L}(\hat{\theta}^{(\tau)}) + e_t, \quad e_t \sim \mathcal{N}(0, \eta I),$$

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

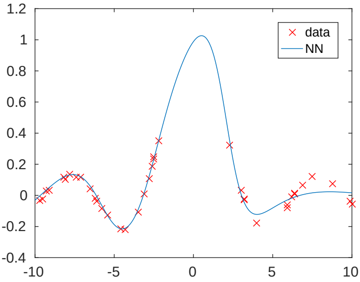
Laplace



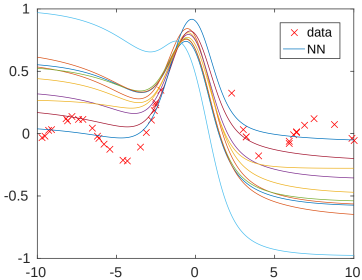




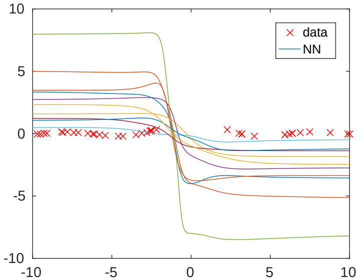
Laplace II



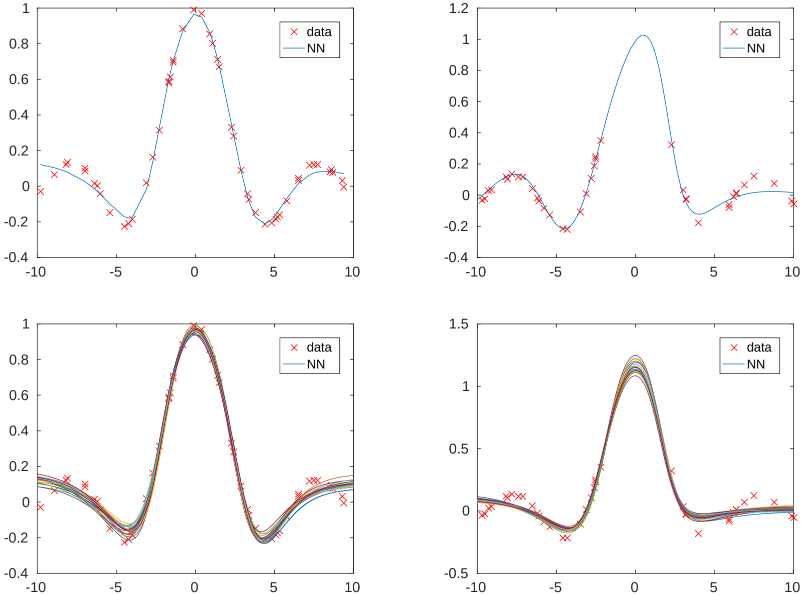
max+0.1std



max+std



Langevin MCMC (tweaked)



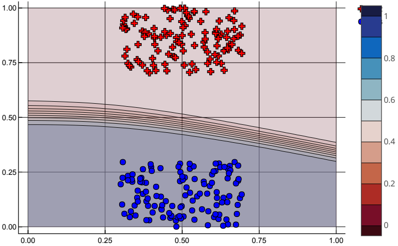
Hamiltonian Monte Carlo

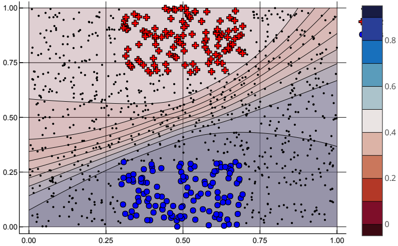
Maximum likelihood

$$p(y|x, \hat{\theta})$$

Average prediction of 500 HMC

$$\frac{1}{N}\sum_{i=1}^{N} p(y|x, \theta^{(i)}),$$





Dropout MC

Standard Network Model:

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

Dropout Network Model:

$$z_i = \sigma_i \left(W_i \left(\xi_i \circ x \right) + b_1 \right),$$
$$y = \sigma_2 \left(w_m (\xi_m \circ z_m) + b_m \right)$$

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):

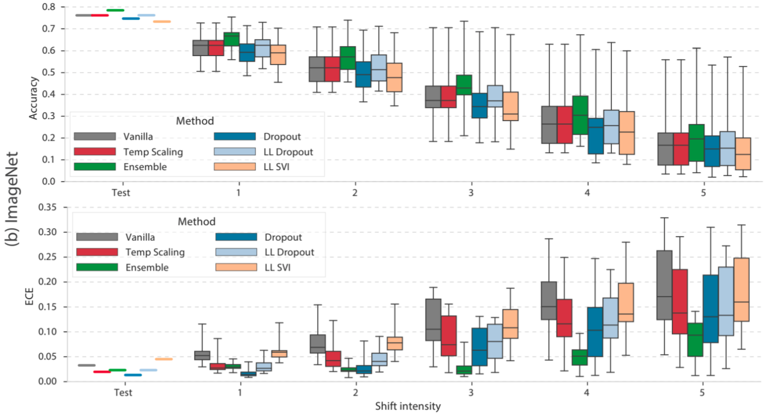
$$\eta^* = \frac{2S}{N}\frac{\dim(\theta)}{\mathrm{tr}(C)}, \text{ or } \qquad H^* = \frac{2S}{N}C^{-1}, \text{ (matrix learning rate)}$$

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

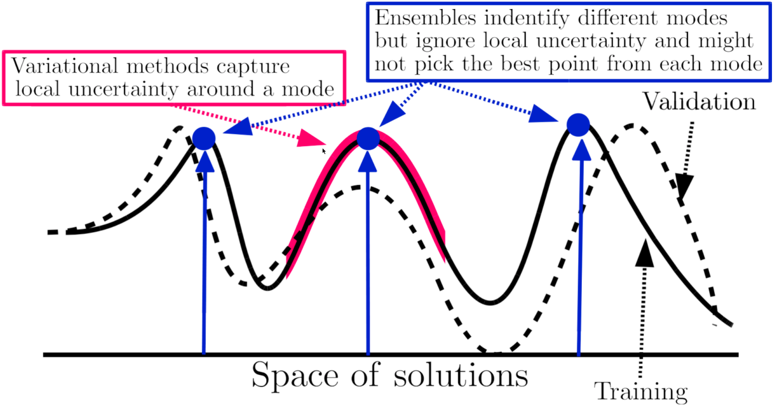
Various methods were compared in (Ovadia, et. al 2019):



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 (10pt)

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