# Stochastic Computation Graphs, and Pathwise Derivative Policy Gradient Methods

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# Stochastic Computation Graphs

# Motivation

- Gradient estimation is at the core of much of modern machine learning
- Backprop is mechanical: this us more freedom to tinker with architectures and loss functions
- RL (and certain probabilistic models) involve components you can't backpropagate through—need REINFORCE-style estimators logprob * advantage
- Often we need a combination of backprop-style and REINFORCE-style gradient estimation
  - RNN policies $\pi(a_t \mid h_t)$, where $h_t = f(h_{t-1}, a_{t-1}, o_t)$
  - Instead of reward, we have a known differentiable function, e.g. classifier with hard attention. Objective = logprob of correct label.
- Each paper to propose such a model provides a new convoluted derivation

# Gradients of Expectations

Want to compute $\nabla_\theta \mathbb{E}[F]$. Where's $\theta$?

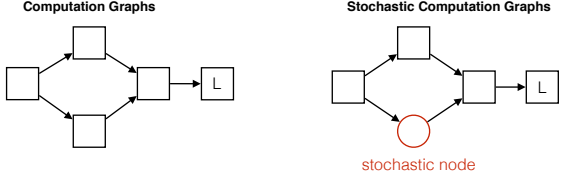
- "Inside" distribution, e.g., $\mathbb{E}_{x\sim p(\cdot\,|\,\theta)}[F(x)]$
  - $\nabla_\theta \mathbb{E}_x[f(x)] = \mathbb{E}_x[f(x)\nabla_\theta \log p_x(x;\ \theta)]$.
  - Score function (SF) estimator
  - Example: REINFORCE policy gradients, where $x$ is the trajectory
- Inside expectation: $\mathbb{E}_{z\sim\mathcal{N}(0,1)}[F(\theta, z)]$

$$\nabla_\theta \mathbb{E}_z[f(x(z,\theta))] = \mathbb{E}_z[\nabla_\theta f(x(z,\theta))].$$

  - Pathwise derivative (PD) estimator
  - Example: neural net with dropout
- Often, we can reparametrize, to change from one form to another
  - Not a property of problem: equivalent ways of writing down the same stochastic process
- What if $F$ depends on $\theta$ in complicated way, affecting distribution and $F$?

# Stochastic Computation Graphs

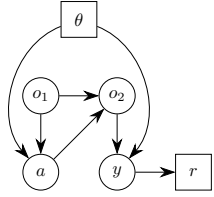
- Stochastic computation graph is a DAG, each node corresponds to a deterministic or stochastic operation
- Can automatically derive unbiased gradient estimators, with variance reduction

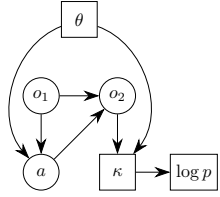



J. Schulman, N. Heess, T. Weber, et al. "Gradient Estimation Using Stochastic Computation Graphs". In: *NIPS*. 2015

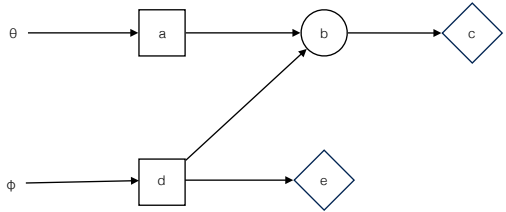
# Example: Hard Attention

- Look at image ($o_1$)
- Determine crop window ($a$)
- Get cropped image ($o_2$)
- Version 1
  - Output label ($y$)
  - Get reward of 1 for correct label
- Version 2
  - Output parameter specifying distribution over label ($\kappa$)
  - Reward = prob or logprob of correct label ($\log p$)



# Abstract Example




- $L = c + e$. Want to compute $\frac{\mathrm{d}}{\mathrm{d}\theta}\mathbb{E}[L]$ and $\frac{\mathrm{d}}{\mathrm{d}\phi}\mathbb{E}[L]$.
- Treat stochastic node $b$) as constants, and introduce losses $\mathit{logprob} * (\mathit{futurecost} - \mathit{optionalbaseline})$ at each stochastic node
- Obtain unbiased gradient estimate by differentiating surrogate:

$$\mathrm{Surrogate}(\theta, \psi) = \underbrace{c + e}_{(1)} + \underbrace{\log p(\hat{b} \mid a, d)\hat{c}}_{(2)}$$

(1): how parameters influence cost through deterministic dependencies

(2): how parameters affect distribution over random variables.

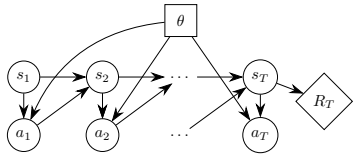
# Results

- General method for calculating gradient estimator
  - Surrogate loss version: each stochastic node gives a loss expression logprob(node value) * (sum of "downstream" costs *treated as constants*). Add these to the sum of costs *treated as variables*.
  - Alternative generalized backprop: as usual, do reverse topological sort. Instead of backpropagating using Jacobian, backpropagate gradlogprob * futurecosts.
- Generalized version of baselines for variance reduction (without bias): logp(node) * (sum of downstream costs treated as constants minus baseline(nondescendents of node))

# Pathwise Derivative Policy Gradient Methods

# Deriving the Policy Gradient, Reparameterized

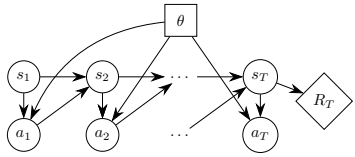
- Episodic MDP:




Want to compute $\nabla_\theta \mathbb{E}[R_T]$. We'll use $\nabla_\theta \log \pi(a_t \mid s_t; \theta)$

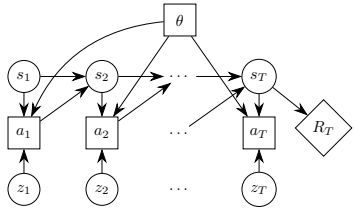
# Deriving the Policy Gradient, Reparameterized

- Episodic MDP:



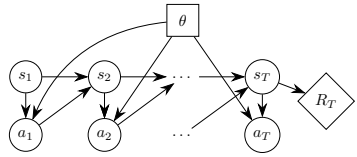

  Want to compute $\nabla_\theta \mathbb{E}[R_T]$. We'll use $\nabla_\theta \log \pi(a_t \mid s_t; \theta)$

- Reparameterize: $a_t = \pi(s_t, z_t; \theta)$. $z_t$ is noise from fixed distribution.



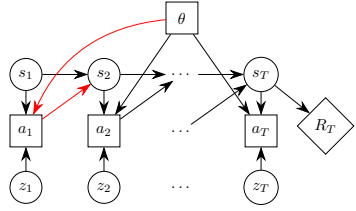
# Deriving the Policy Gradient, Reparameterized

- Episodic MDP:



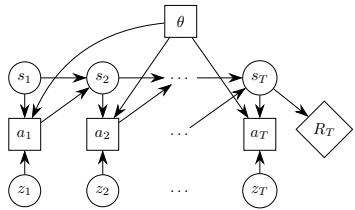

  Want to compute $\nabla_\theta \mathbb{E}[R_T]$. We'll use $\nabla_\theta \log \pi(a_t \mid s_t; \theta)$

- Reparameterize: $a_t = \pi(s_t, z_t; \theta)$. $z_t$ is noise from fixed distribution.




- Only works if $P(s_2 \mid s_1, a_1)$ is known $\ddot{\frown}$

# Using a $Q$-function




$$\frac{\mathrm{d}}{\mathrm{d}\theta}\mathbb{E}\left[R_T\right] = \mathbb{E}\left[\sum_{t=1}^{T}\frac{\mathrm{d}R_T}{\mathrm{d}a_t}\frac{\mathrm{d}a_t}{\mathrm{d}\theta}\right] = \mathbb{E}\left[\sum_{t=1}^{T}\frac{\mathrm{d}}{\mathrm{d}a_t}\mathbb{E}\left[R_T \mid a_t\right]\frac{\mathrm{d}a_t}{\mathrm{d}\theta}\right]$$

$$= \mathbb{E}\left[\sum_{t=1}^{T}\frac{\mathrm{d}Q(s_t, a_t)}{\mathrm{d}a_t}\frac{\mathrm{d}a_t}{\mathrm{d}\theta}\right] = \mathbb{E}\left[\sum_{t=1}^{T}\frac{\mathrm{d}}{\mathrm{d}\theta}Q(s_t, \pi(s_t, z_t; \theta))\right]$$

# SVG(0) Algorithm

- Learn $Q_\phi$ to approximate $Q^{\pi,\gamma}$, and use it to compute gradient estimates.

N. Heess, G. Wayne, D. Silver, et al. "Learning continuous control policies by stochastic value gradients". In: *NIPS*. 2015

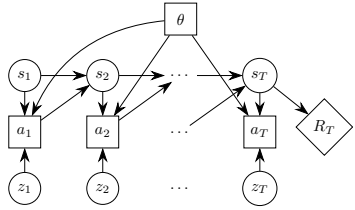
# SVG(0) Algorithm

- Learn $Q_\phi$ to approximate $Q^{\pi,\gamma}$, and use it to compute gradient estimates.
- Pseudocode:

  **for** iteration$=1, 2, \ldots$ **do**
    Execute policy $\pi_\theta$ to collect $T$ timesteps of data
    Update $\pi_\theta$ using $g \propto \nabla_\theta \sum_{t=1}^{T} Q(s_t, \pi(s_t, z_t; \theta))$
    Update $Q_\phi$ using $g \propto \nabla_\phi \sum_{t=1}^{T} (Q_\phi(s_t, a_t) - \hat{Q}_t)^2$, e.g. with TD($\lambda$)
  **end for**

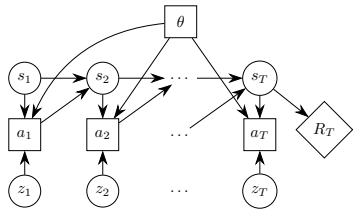
N. Heess, G. Wayne, D. Silver, et al. "Learning continuous control policies by stochastic value gradients". In: *NIPS*. 2015

# SVG(1) Algorithm




- Instead of learning $Q$, we learn
  - State-value function $V \approx V^{\pi,\gamma}$
  - Dynamics model $f$, approximating $s_{t+1} = f(s_t, a_t) + \zeta_t$
- Given transition $(s_t, a_t, s_{t+1})$, infer $\zeta_t = s_{t+1} - f(s_t, a_t)$
- $Q(s_t, a_t) = \mathbb{E}\left[r_t + \gamma V(s_{t+1})\right] = \mathbb{E}\left[r_t + \gamma V(f(s_t, a_t) + \zeta_t)\right]$, and $a_t = \pi(s_t, \theta, \zeta_t)$

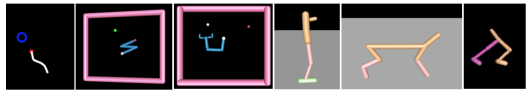
# SVG($\infty$) Algorithm



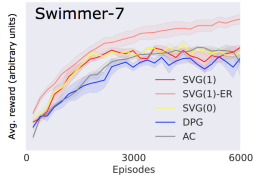

- Just learn dynamics model $f$
- Given whole trajectory, infer all noise variables
- Freeze all policy and dynamics noise, differentiate through entire deterministic computation graph

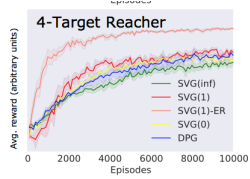
# SVG Results

- Applied to 2D robotics tasks



- Overall: different gradient estimators behave similarly




N. Heess, G. Wayne, D. Silver, et al. "Learning continuous control policies by stochastic value gradients". In: *NIPS*. 2015

# Deterministic Policy Gradient

- For Gaussian actions, variance of score function policy gradient estimator goes to infinity as variance goes to zero
- But SVG(0) gradient is fine when $\sigma \to 0$

$$\nabla_\theta \sum_t Q(s_t, \pi(s_t, \theta, \zeta_t))$$

- Problem: there's no exploration.
- Solution: add noise to the policy, but estimate $Q$ with TD(0), so it's valid off-policy
- Policy gradient is a little biased (even with $Q = Q^\pi$), but only because state distribution is off—it gets the right gradient at every state

D. Silver, G. Lever, N. Heess, et al. "Deterministic policy gradient algorithms". In: *ICML*. 2014

# Deep Deterministic Policy Gradient

- Incorporate replay buffer and target network ideas from DQN for increased stability

T. P. Lillicrap, J. J. Hunt, A. Pritzel, et al. "Continuous control with deep reinforcement learning". In: *ICLR* (2015).

# Deep Deterministic Policy Gradient

- Incorporate replay buffer and target network ideas from DQN for increased stability
- Use lagged (Polyak-averaging) version of $Q_\phi$ and $\pi_\theta$ for fitting $Q_\phi$ (towards $Q^{\pi,\gamma}$) with TD(0)

$$\hat{Q}_t = r_t + \gamma Q_{\phi'}(s_{t+1}, \pi(s_{t+1}; \theta'))$$

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# Deep Deterministic Policy Gradient

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$$\hat{Q}_t = r_t + \gamma Q_{\phi'}(s_{t+1}, \pi(s_{t+1}; \theta'))$$

- Pseudocode:

**for** iteration$=1, 2, \ldots$ **do**
  Act for several timesteps, add data to replay buffer
  Sample minibatch
  Update $\pi_\theta$ using $g \propto \nabla_\theta \sum_{t=1}^{T} Q(s_t, \pi(s_t, z_t; \theta))$
  Update $Q_\phi$ using $g \propto \nabla_\phi \sum_{t=1}^{T} (Q_\phi(s_t, a_t) - \hat{Q}_t)^2$,
**end for**

T. P. Lillicrap, J. J. Hunt, A. Pritzel, et al. "Continuous control with deep reinforcement learning". In: *ICLR* (2015).

# DDPG Results

Applied to 2D and 3D robotics tasks and driving with pixel input

T. P. Lillicrap, J. J. Hunt, A. Pritzel, et al. "Continuous control with deep reinforcement learning". In: *ICLR* (2015).

# Policy Gradient Methods: Comparison

| Task | Random | REINFORCE | TNPG | RWR | REPS | TRPO | CEM | CMA-ES | DDPG |
|---|---|---|---|---|---|---|---|---|---|
| Cart-Pole Balancing | 77.1 ± 0.0 | 4693.7 ± 14.0 | **3986.4 ± 748.9** | **4861.5 ± 12.3** | 565.6 ± 137.6 | **4869.8 ± 37.6** | 4815.4 ± 4.8 | 2440.4 ± 568.3 | 4634.4 ± 87.8 |
| Inverted Pendulum* | −153.4 ± 0.2 | 13.4 ± 18.0 | **209.7 ± 55.5** | 84.7 ± 13.8 | −113.3 ± 4.6 | **247.2 ± 76.1** | 38.2 ± 25.7 | −40.1 ± 5.7 | 40.0 ± 244.6 |
| Mountain Car | −415.4 ± 0.0 | −67.1 ± 1.0 | **-66.5 ± 4.5** | −79.4 ± 1.1 | −275.6 ± 166.3 | **-61.7 ± 0.9** | −66.0 ± 2.4 | −85.0 ± 7.7 | −288.4 ± 170.3 |
| Acrobot | −1904.5 ± 1.0 | −508.1 ± 91.0 | −395.8 ± 121.2 | −352.7 ± 35.9 | −1001.5 ± 10.8 | −326.0 ± 24.4 | −436.8 ± 14.7 | −785.6 ± 13.1 | **-223.6 ± 5.8** |
| Double Inverted Pendulum* | 149.7 ± 0.1 | 4116.5 ± 65.2 | **4455.4 ± 37.6** | 3614.8 ± 368.1 | 446.7 ± 114.8 | **4412.4 ± 50.4** | 2566.2 ± 178.9 | 1576.1 ± 51.3 | 2863.4 ± 154.0 |
| Swimmer* | −1.7 ± 0.1 | 92.3 ± 0.1 | **96.0 ± 0.2** | 60.7 ± 5.5 | 3.8 ± 3.3 | **96.0 ± 0.2** | 68.8 ± 2.4 | 64.9 ± 1.4 | 85.8 ± 1.8 |
| Hopper | 8.4 ± 0.0 | 714.0 ± 29.3 | **1155.1 ± 57.9** | 553.2 ± 71.0 | 86.7 ± 17.6 | **1183.3 ± 150.0** | 63.1 ± 7.8 | 20.3 ± 14.3 | 267.1 ± 43.5 |
| 2D Walker | −1.7 ± 0.0 | 506.5 ± 78.8 | **1302.6 ± 108.2** | 136.0 ± 15.9 | −37.0 ± 38.1 | **1353.8 ± 85.0** | 84.5 ± 19.2 | 77.1 ± 24.3 | 318.4 ± 181.6 |
| Half-Cheetah | −90.8 ± 0.3 | 1183.1 ± 69.2 | **1729.5 ± 184.6** | 376.1 ± 28.2 | 34.5 ± 38.0 | **1914.0 ± 120.1** | 330.4 ± 274.8 | 441.3 ± 107.6 | **2148.6 ± 702.7** |
| Ant* | 13.4 ± 0.7 | 548.3 ± 55.5 | **706.0 ± 127.7** | 37.6 ± 3.1 | 39.0 ± 9.8 | **730.2 ± 61.3** | 49.2 ± 5.9 | 17.8 ± 15.5 | 326.2 ± 20.8 |
| Simple Humanoid | 41.5 ± 0.2 | 128.1 ± 34.0 | **255.0 ± 24.5** | 93.3 ± 17.4 | 28.3 ± 4.7 | **269.7 ± 40.3** | 60.6 ± 12.9 | 28.7 ± 3.9 | 99.4 ± 28.1 |
| Full Humanoid | 13.2 ± 0.1 | 262.2 ± 10.5 | **288.4 ± 25.2** | 46.7 ± 5.6 | 41.7 ± 6.1 | **287.9 ± 23.4** | 36.9 ± 2.9 | N/A ± N/A | 119.0 ± 31.2 |
| Cart-Pole Balancing (LS)* | 77.1 ± 0.0 | 420.9 ± 265.5 | **945.1 ± 27.8** | 68.9 ± 1.5 | 898.1 ± 22.1 | **960.2 ± 46.0** | 227.0 ± 223.0 | 68.0 ± 1.6 | |
| Inverted Pendulum (LS) | −122.1 ± 0.1 | −13.4 ± 3.2 | **0.7 ± 6.1** | −107.4 ± 0.2 | −87.2 ± 8.0 | **4.5 ± 4.1** | −81.2 ± 33.2 | −62.4 ± 3.4 | |
| Mountain Car (LS) | −83.0 ± 0.0 | −81.2 ± 0.6 | **-65.7 ± 9.0** | −81.7 ± 0.1 | −82.6 ± 0.4 | **-64.2 ± 9.5** | **-68.9 ± 1.3** | **-73.2 ± 0.6** | |
| Acrobot (LS)* | −393.2 ± 0.0 | −128.9 ± 11.6 | **-84.6 ± 2.9** | −235.9 ± 5.3 | −379.5 ± 1.4 | **-83.3 ± 9.9** | −149.5 ± 15.3 | −159.9 ± 7.5 | |
| Cart-Pole Balancing (NO)* | 101.4 ± 0.1 | 616.0 ± 210.8 | **916.3 ± 23.0** | 93.8 ± 1.2 | 99.6 ± 7.2 | 606.2 ± 122.2 | 181.4 ± 32.1 | 104.4 ± 16.0 | |
| Inverted Pendulum (NO) | −122.2 ± 0.1 | 6.5 ± 1.1 | **11.5 ± 0.5** | −110.0 ± 1.4 | −119.3 ± 4.2 | **10.4 ± 2.2** | −55.6 ± 16.7 | −80.3 ± 2.8 | |
| Mountain Car (NO) | −83.0 ± 0.0 | −74.7 ± 7.8 | **-64.5 ± 8.6** | −81.7 ± 0.1 | −82.9 ± 0.1 | **-60.2 ± 2.0** | −67.4 ± 1.4 | −73.5 ± 0.5 | |
| Acrobot (NO)* | −393.5 ± 0.0 | **-186.7 ± 31.3** | **-164.5 ± 13.4** | −233.1 ± 0.4 | −258.5 ± 14.0 | **-149.6 ± 8.6** | −213.4 ± 6.3 | −236.6 ± 6.2 | |
| Cart-Pole Balancing (SI)* | 76.3 ± 0.1 | 431.7 ± 274.1 | **980.5 ± 7.3** | 69.0 ± 2.8 | 702.4 ± 196.4 | **980.3 ± 5.1** | 746.6 ± 93.2 | 71.6 ± 2.9 | |
| Inverted Pendulum (SI) | −121.8 ± 0.2 | −5.3 ± 5.6 | **14.8 ± 1.7** | −108.7 ± 4.7 | −92.8 ± 23.9 | **14.1 ± 0.9** | −51.8 ± 10.6 | −63.1 ± 4.8 | |
| Mountain Car (SI) | −82.7 ± 0.0 | −63.9 ± 0.2 | **-61.8 ± 0.4** | −81.4 ± 0.1 | −80.7 ± 2.3 | **-61.6 ± 0.4** | −63.9 ± 1.0 | −66.9 ± 0.6 | |
| Acrobot (SI)* | −387.8 ± 1.0 | **-169.1 ± 32.3** | **-156.6 ± 38.9** | −233.2 ± 2.6 | −216.1 ± 7.7 | **-170.9 ± 40.3** | −250.2 ± 13.7 | −245.0 ± 5.5 | |
| Swimmer + Gathering | 0.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 |
| Ant + Gathering | −5.8 ± 5.0 | −0.1 ± 0.1 | −0.4 ± 0.1 | −5.5 ± 0.5 | −6.7 ± 0.7 | −0.4 ± 0.0 | −4.7 ± 0.7 | N/A ± N/A | −0.3 ± 0.3 |
| Swimmer + Maze | 0.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 |
| Ant + Maze | 0.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | N/A ± N/A | 0.0 ± 0.0 |

Y. Duan, X. Chen, R. Houthooft, et al. "Benchmarking Deep Reinforcement Learning for Continuous Control". In: *ICML* (2016).